

# Protein Visualization

PhD. Pablo Ricardo Arantes

Riverside, April 18th 2024



# EDUCATION

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2007-2012 Bachelor of Pharmacy  
UFRGS – Porto Alegre, BR  
Supervisor: Dr. Hugo Verli

2013-2014 M. Sc. in Cellular &  
Molecular Biology  
PPGBCM - UFRGS – Porto Alegre, BR  
Supervisor: Dr. Hugo Verli

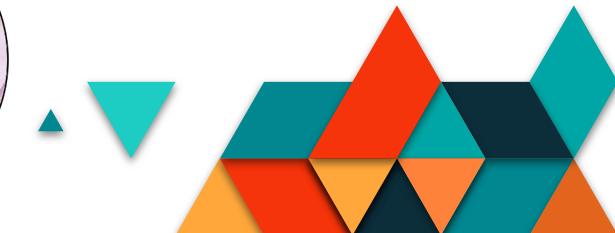
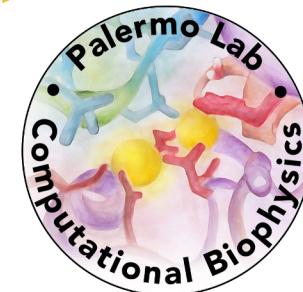
2014-2018 PhD in Cellular &  
Molecular Biology  
PPGBCM - UFRGS – Porto Alegre, BR  
Supervisor: Dr. Hugo Verli

2018-2019 Postdoctoral Researcher  
PPGBio - UFCSPA - Porto Alegre, BR  
Supervisor: Dr. Dinara Jaqueline Moura

2019-2023 Postdoctoral Researcher  
University of California, Riverside  
Supervisor: Dr. Giulia Palermo



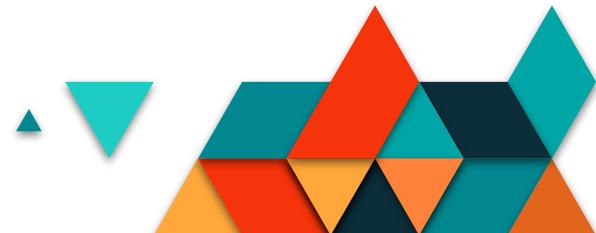
Universidade Federal de Ciências da Saúde  
de Porto Alegre



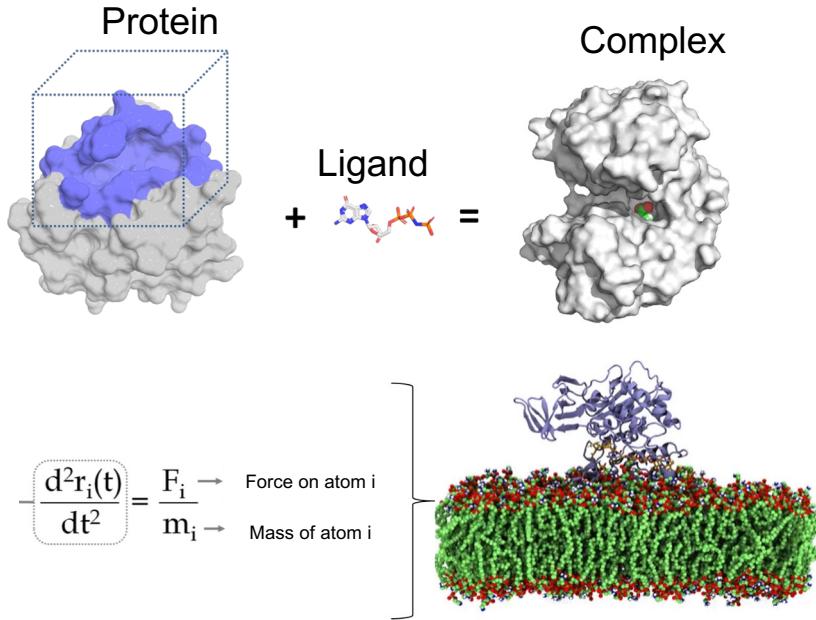
# Slides

## Jupyter Notebooks examples

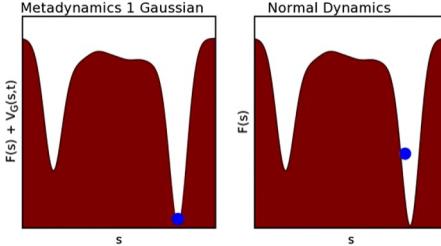
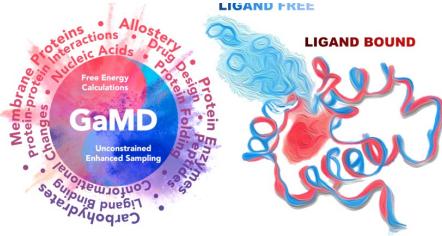
<https://github.com/pablo-arantes/BIEN165>



# COMPUTATIONAL CHEMISTRY



$$\text{Acceleration of atom } i = \frac{d^2\mathbf{r}_i(t)}{dt^2} = \frac{\mathbf{F}_i}{m_i} \rightarrow \begin{array}{l} \text{Force on atom } i \\ \text{Mass of atom } i \end{array}$$



## MOLECULAR MODELING

**Programs:** AlphaFold2; Modeller; Rosetta; I-Tasser; Phyre 2;

# MOLECULAR DOCKING - CHEMIOINFORMATICS

**Programs:** Autodock Vina; Autodock; DockThor (Brazil); RDKit; TorchANI

# MOLECULAR DYNAMICS (Molecular Mechanics)

**Programs:** Amber; OpenMM; GROMACS; NAMD;

# ENHANCED SAMPLING

**Programs:** Amber; GROMACS; PLUMED; GaMD;



# Micro x Macromolecules

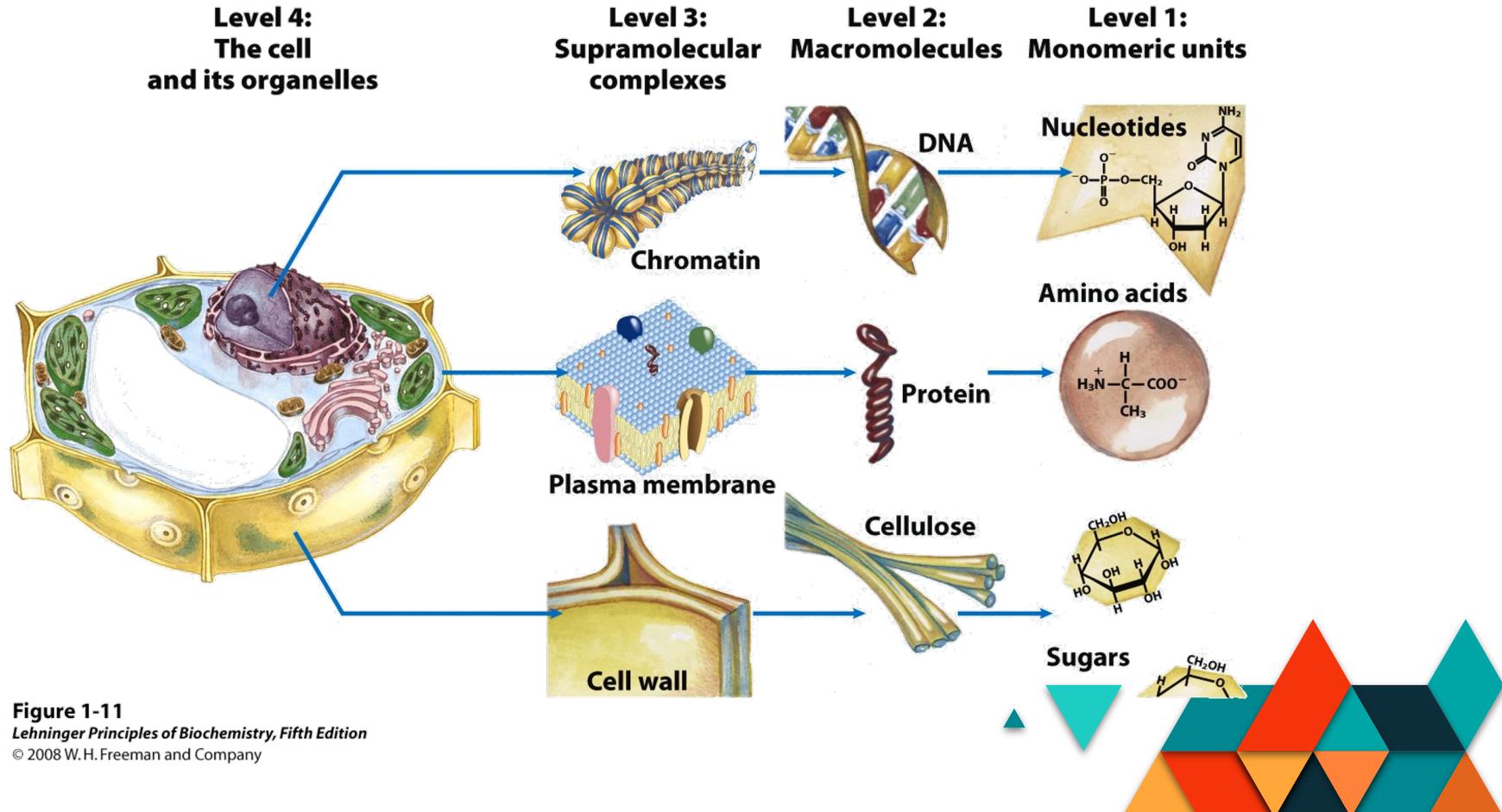
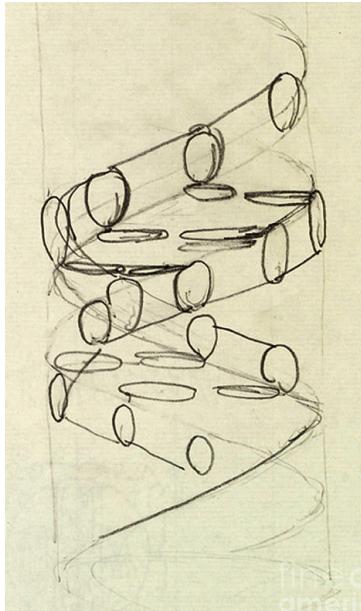
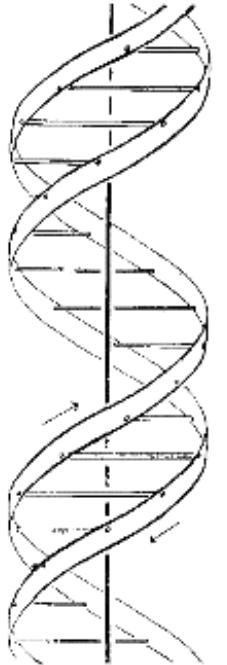


Figure 1-11

*Lehninger Principles of Biochemistry, Fifth Edition*  
© 2008 W.H. Freeman and Company

# Micro x Macromolecules



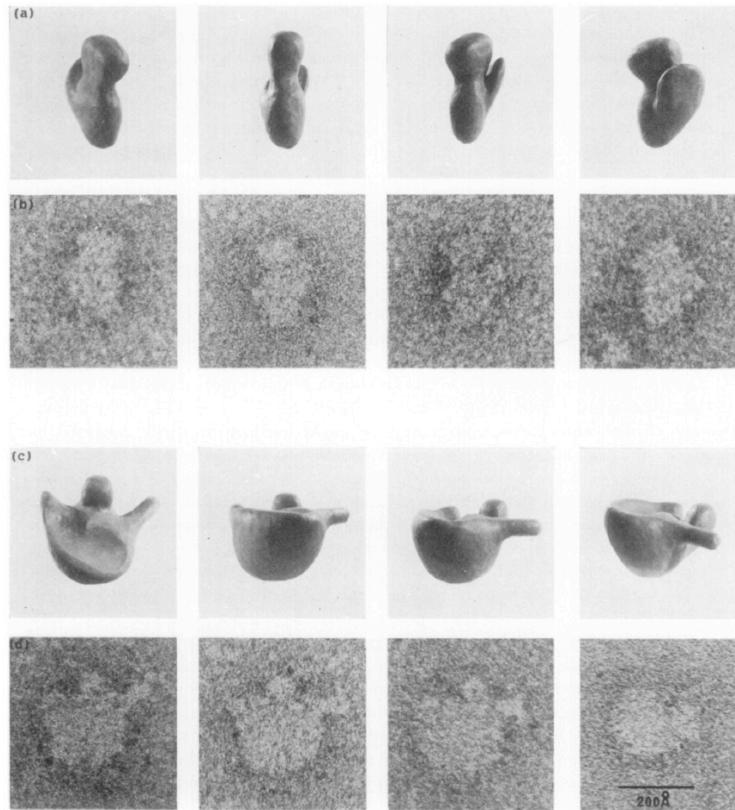
This figure is purely diagrammatic. The two ribbons symbolize the two phosphate-sugar chains, and the horizontal rods the pairs of bases holding the chains together. The vertical line marks the fibre axis

**“To understand, we need to see”**  
(Liljas et al., 2009)

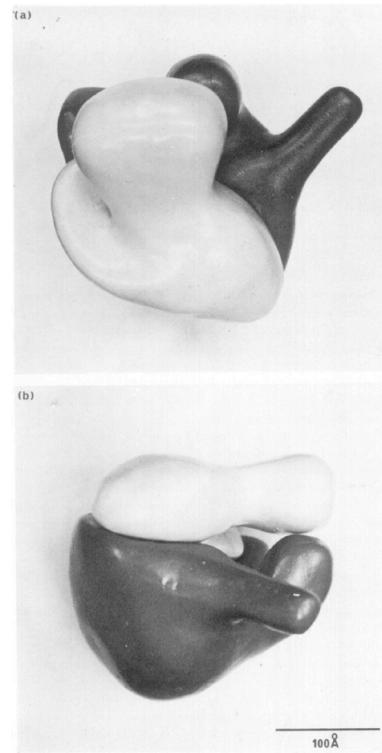
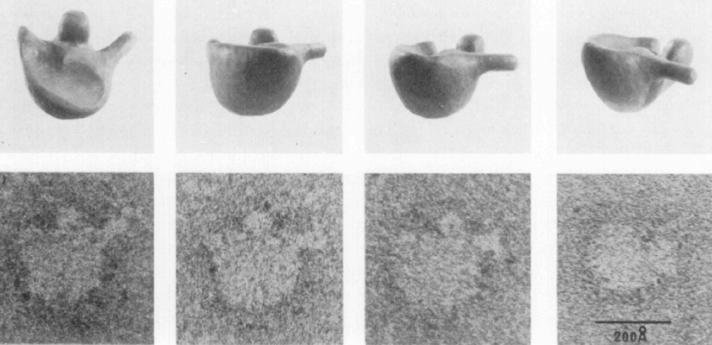
**“Unfortunately, we cannot accurately describe at the chemical level how a molecule functions unless we know first its structure”**

(J. Watson, 1964)



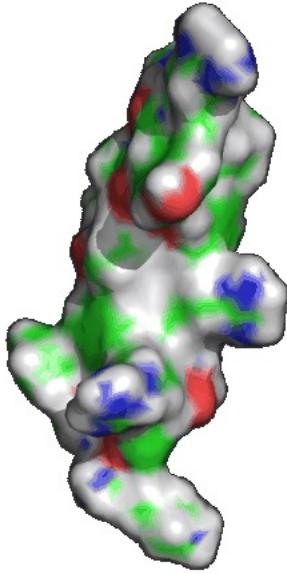


(c)

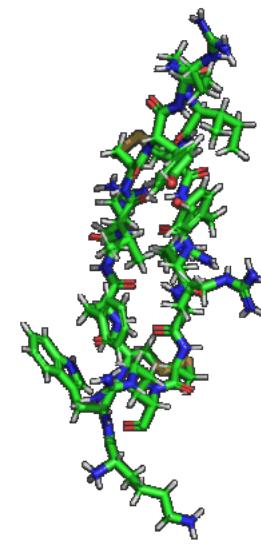
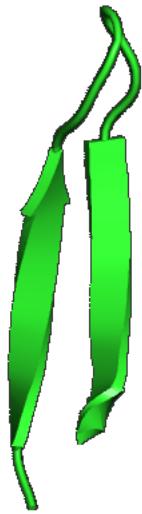


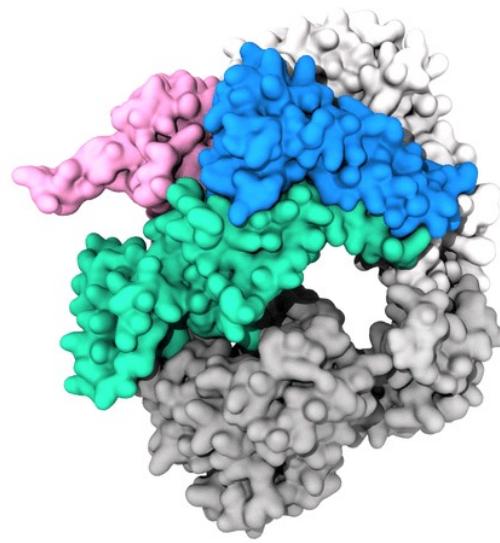
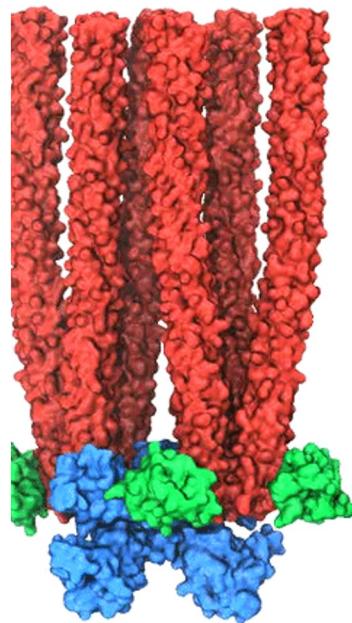
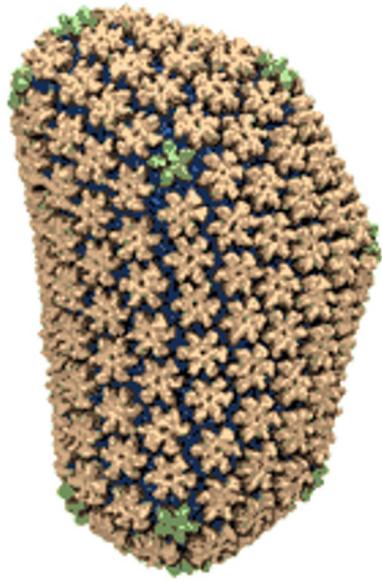
(b)





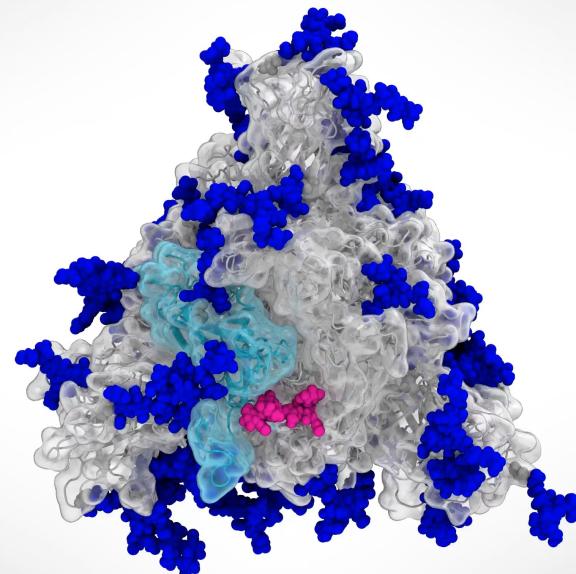
PDB id 1W00





# Closed Spike

*Top view*

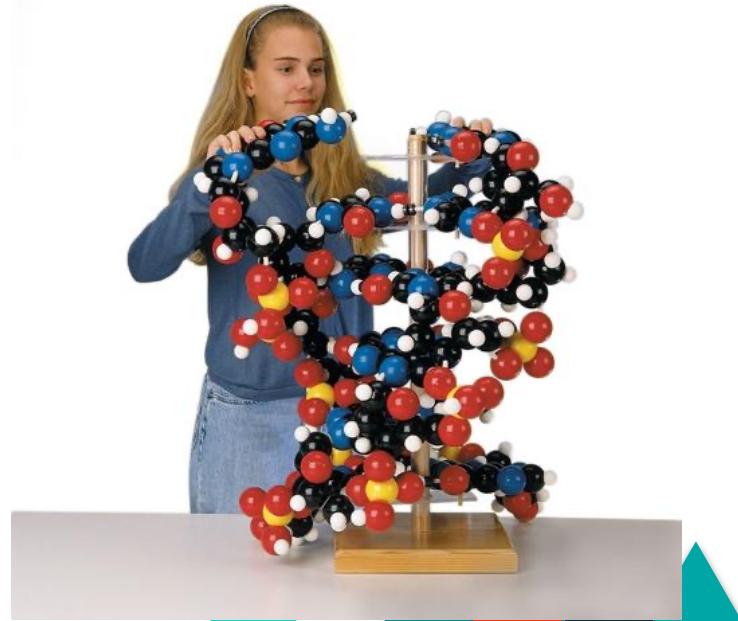


MOVIE BY L. CASALINO

T. SZTAIN, S.-H. AHN et al.  
AMARO LAB (UCSD)  
CHONG LAB (PITT)

Supercomputing-driven simulations depict the glycan N343 (magenta) acting as a molecular crowbar to pry open the SARS-CoV-2 spike's receptor binding domain, or RBD (cyan), from a "down" to an "up" position. **Nature Chemistry, 2021.**

# Micro x Macromolecules



# Micro x Macromolecules

## Big Bang Theory DNA Model-Fully Assembled

SKU: 62122-36

Indigo Instruments

"The Big Bang Theory" DNA Model

Often Imitated - Never Duplicated.  
We are the Original.

Copyright © Indigo® Instruments. All Rights Reserved

\$1,995.00USD Each

Qty:

1

ADD TO CART

Add to Wish List

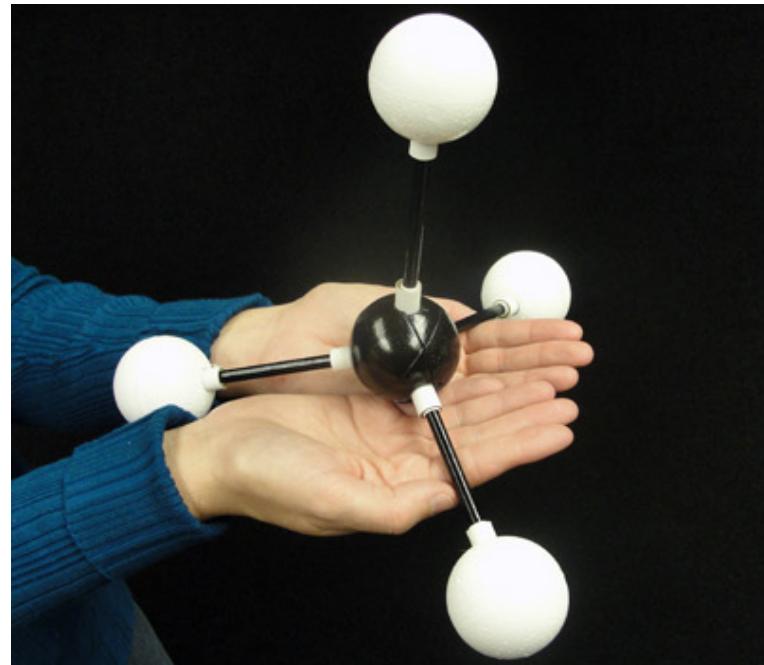
[5] 2 Reviews | [Write a Review](#)

The Indigo® 36 base pair DNA model is an expanded version of the one appearing on the Big Bang Theory. The latter was built with 2 of our [17 base pair versions](#) while this one has 2 extra base pairs. It stands nearly nearly 2m tall and is as accurate as the original as demonstrated by the fit with the custom Indigo® [alpha helix model](#). Note that the model now comes with a larger, more stable base than is shown in the image.

- Delivery in North America is typically ~2 weeks.
- Ask us about our [semi-assembled version](#) to save on overseas air freight charges.
- [Working on Biochemistry of Aging?](#) Additional parts available to show Methylation of DNA Cytosine Nucleoside. Contact us to add these parts to your DNA model order.
- Studies in Aging & one of our very low cost [DNA models](#) could be an interesting science fair project
- A history of the [Indigo® Big Bang Theory DNA Model](#)
- 18,014,398,509,482,000 variations. Buy yours while supplies last



# Micro x Macromolecules



[nature](#) > [nature methods](#) > [review articles](#) > article

Review Article | Published: 01 March 2010

## Visualization of macromolecular structures

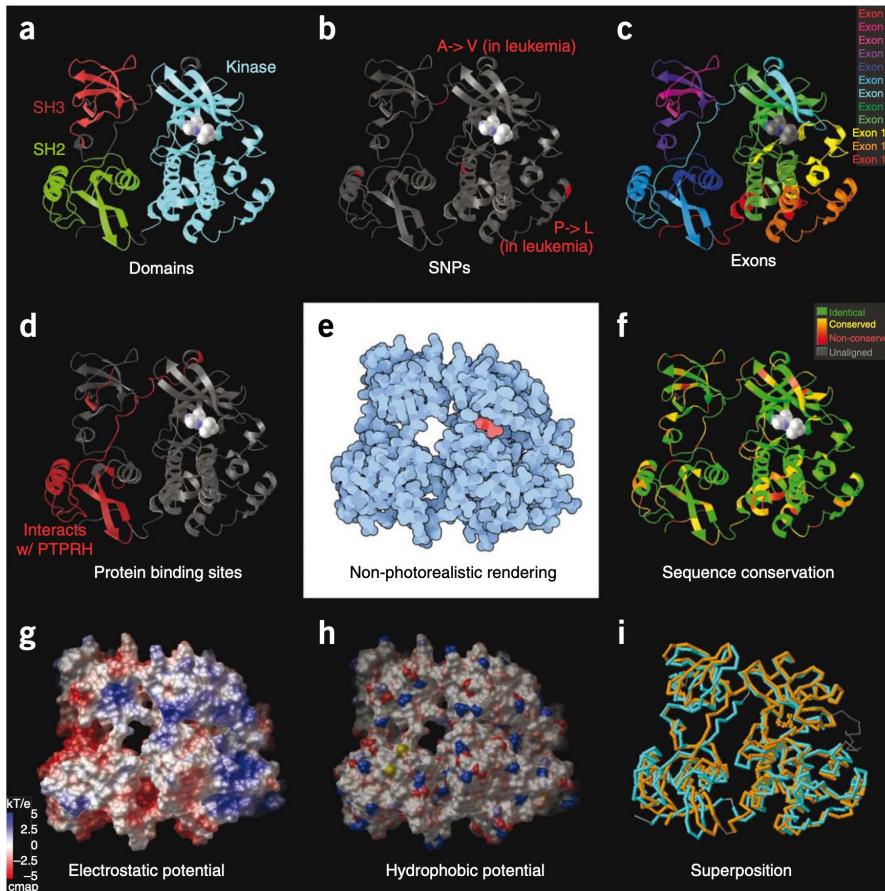
[Seán I O'Donoghue](#)  , [David S Goodsell](#), [Achilleas S Frangakis](#), [Fabrice Jossinet](#), [Roman A Laskowski](#),  
[Michael Nilges](#), [Helen R Saibil](#), [Andrea Schafferhans](#), [Rebecca C Wade](#), [Eric Westhof](#) & [Arthur J Olson](#)

[Nature Methods](#) 7, S42–S55 (2010) | [Cite this article](#)

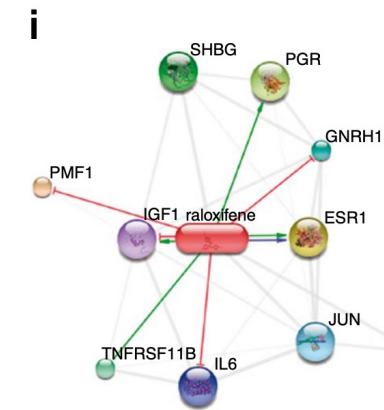
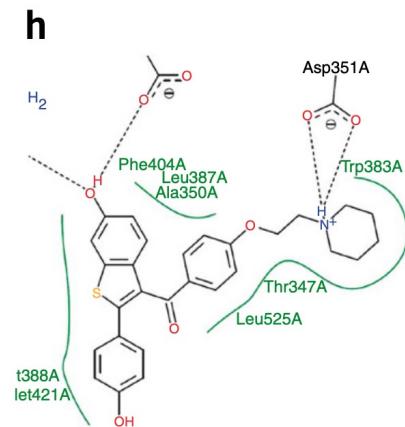
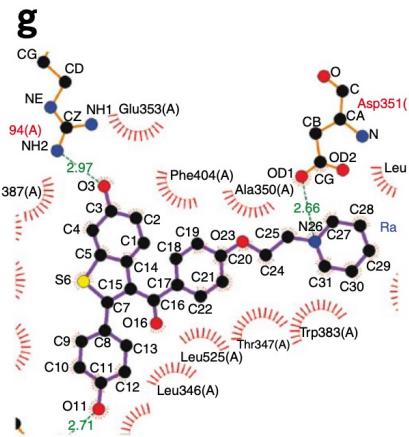
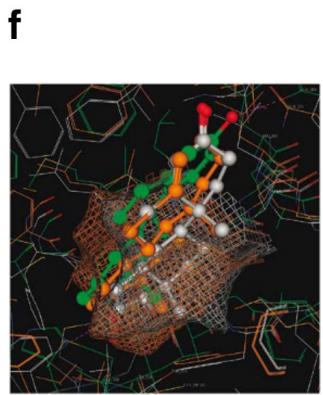
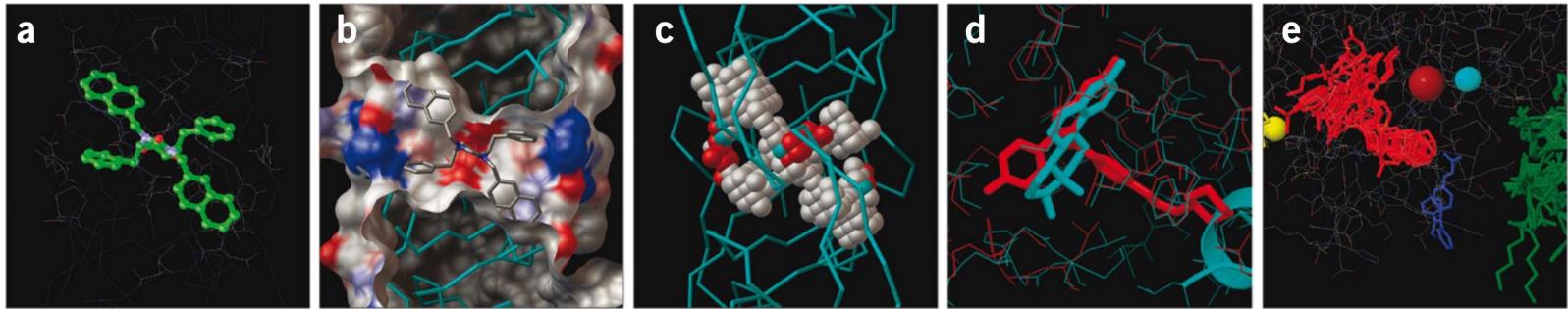
9210 Accesses | 114 Citations | 14 Altmetric | [Metrics](#)

doi:10.1038/nmeth.1427





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**Table 1 |** Selected resources for finding and visualizing macromolecules

Name	Cost	OS	Description	URL
<b>Stand-alone</b>				
Amira	\$	Win, Mac, Linux	Combines many different methods and scripting (EDM, MRI, optical)	<a href="http://www.amiravis.com/">http://www.amiravis.com/</a>
Cn3D <sup>17</sup>	Free	Win, Mac, Linux	Integrated sequence alignment view; embeddable	<a href="http://tinyurl.com/Cn3D-NCBI/">http://tinyurl.com/Cn3D-NCBI/</a>
Chime	Free	Win	Widely used; structure editing; electrostatic maps; embeddable	<a href="http://tinyurl.com/chime-pro/">http://tinyurl.com/chime-pro/</a>
Chimera <sup>16</sup>	Free	Win, Mac, Linux	Popular; integrated sequence alignment viewer (EDM, MD)	<a href="http://www.cgl.ucsf.edu/chimera/">http://www.cgl.ucsf.edu/chimera/</a>
DS Visualizer	Free	Win, Mac, Linux	Free version of Accelrys's powerful viewer/editor program	<a href="http://tinyurl.com/DSVisualizer/">http://tinyurl.com/DSVisualizer/</a>
ICM-Browser	Free	Win, Mac, Linux	High quality images; integrates with sequence alignment viewer	<a href="http://tinyurl.com/icm-browser/">http://tinyurl.com/icm-browser/</a>
IMOD <sup>109</sup>	Free	Win, Mac, Linux	Tomogram alignment, display, segmentation (EDM, optical)	<a href="http://bio3d.colorado.edu/imod/">http://bio3d.colorado.edu/imod/</a>
Jmol	Free	Win, Mac, Linux	Widely used; embeddable	<a href="http://www.jmol.org/">http://www.jmol.org/</a>
KiNG	Free	Win, Mac, Linux	Generic tool for creating 'kinemages'	<a href="http://tinyurl.com/KINGapp/">http://tinyurl.com/KINGapp/</a>
Mage <sup>6</sup>	Free	Win, Mac, Linux	Generic tool for creating 'kinemages'; allows structure editing	<a href="http://tinyurl.com/kinemage/">http://tinyurl.com/kinemage/</a>
MOE	\$	Win, Mac, Linux	Integrated multifunctional suite; useful for drug design (MM)	<a href="http://www.chemcomp.com/">http://www.chemcomp.com/</a>
Molscript <sup>23</sup>	Free	Unix	Useful for preparing manuscript images	<a href="http://www.avatar.se/molscript/">http://www.avatar.se/molscript/</a>
MolSurfer	Free	Win, Mac, Linux	Shows macromolecular interfaces, for example, by electrostatic potential	<a href="http://tinyurl.com/molsurfer/">http://tinyurl.com/molsurfer/</a>
MOLMOL <sup>35</sup>	Free	Win, Mac, Linux	Many features, particularly suited for NMR structures	<a href="http://tinyurl.com/molmol1/">http://tinyurl.com/molmol1/</a>
OpenAstexViewer <sup>18</sup>	Free	Win, Mac, Linux	Embedded in many PDBe (see below) services	<a href="http://www.openastexviewer.net/">http://www.openastexviewer.net/</a>
ProSAT2 (ref. 31)	Free	Win, Mac, Linux	Displays sequence features on three-dimensional structure	<a href="http://tinyurl.com/ProSAT2/">http://tinyurl.com/ProSAT2/</a>
PMV <sup>25</sup>	Free	Win, Mac, Linux	Dynamically extensible; multiple structures, large assemblies (MM)	<a href="http://tinyurl.com/PMV-MGL/">http://tinyurl.com/PMV-MGL/</a>
PyMOL	Free	Win, Mac, Linux	Widely used; embeddable; high-quality images (EDM, MM)	<a href="http://www.pymol.org/">http://www.pymol.org/</a>
RasMol <sup>110</sup>	Free	Win, Mac, Linux	Widely used; fast; scripting	<a href="http://www.rasmol.org/">http://www.rasmol.org/</a>
Raster3D <sup>24</sup>	Free	Win, Mac, Linux	High-quality, photorealistic rendering	<a href="http://tinyurl.com/raster3d/">http://tinyurl.com/raster3d/</a>
SPICE <sup>27</sup>	Free	Win, Mac, Linux	Adds DAS features to three-dimensional structures	<a href="http://tinyurl.com/spice-browser/">http://tinyurl.com/spice-browser/</a>
STRAP <sup>19</sup>	Free	Win, Mac, Linux	Editor for structural alignments of proteins (HM)	<a href="http://tinyurl.com/STRAP1/">http://tinyurl.com/STRAP1/</a>
Swiss-PdbViewer <sup>20</sup>	Free	Win, Mac, Linux	Integrated sequence view (EDM, MM)	<a href="http://spdbv.vital-it.ch/">http://spdbv.vital-it.ch/</a>
SYBYL	\$	Win, Mac, Linux	Popular molecular modeling tool (MM)	<a href="http://tinyurl.com/triposSYBYL/">http://tinyurl.com/triposSYBYL/</a>
VMD <sup>26*</sup>	Free	Win, Mac, Linux	Widely used; extensible, many add-ons (EDM, MD, MM, NMR)	<a href="http://tinyurl.com/VMD-viewer/">http://tinyurl.com/VMD-viewer/</a>
WHAT IF <sup>42</sup>	\$	Win, Mac, Linux	Powerful features; good support (EDM, HM, MM)	<a href="http://swift.cmbi.ru.nl/whatif/">http://swift.cmbi.ru.nl/whatif/</a>
Yasara	Free	Win, Mac, Linux	Innovative 'virtual reality' graphical user-interface (EDM, MM, NMR)	<a href="http://www.yasara.org/">http://www.yasara.org/</a>

doi:10.1038/nmeth.1427



## Web-based

CAME	Free	Assesses structure quality (ProSA-Web <sup>111</sup> ); finds structural homologs	<a href="http://www.came.sbg.ac.at/">http://www.came.sbg.ac.at/</a>
EMDB	Free	Central repository for electron microscopy density maps	<a href="http://emdatabank.org/">http://emdatabank.org/</a>
Entrez Structure	Free	Finds related structures for a sequence	<a href="http://tinyurl.com/entrez3d/">http://tinyurl.com/entrez3d/</a>
FirstGlance	Free	Useful for a first impression of a structure	<a href="http://firstglance.jmol.org/">http://firstglance.jmol.org/</a>
JenaLib <sup>28</sup>	Free	Displays sequence features on three-dimensional structure	<a href="http://tinyurl.com/JenaLib/">http://tinyurl.com/JenaLib/</a>
NDB <sup>68</sup>	Free	Central repository for nucleic acid structures	<a href="http://ndbserver.rutgers.edu/">http://ndbserver.rutgers.edu/</a>
PDBe	Free	European branch of wwPDB (formerly MSD); many services	<a href="http://www.ebi.ac.uk/pdbe/">http://www.ebi.ac.uk/pdbe/</a>
PDBsum <sup>29</sup>	Free	Pictorial structural annotations	<a href="http://www.ebi.ac.uk/pdbsum/">http://www.ebi.ac.uk/pdbsum/</a>
PISA <sup>33</sup>	Free	Predicts biologically relevant quaternary structure	<a href="http://tinyurl.com/piserver/">http://tinyurl.com/piserver/</a>
Relibase <sup>58,59</sup>	Free/\$	Finds similar ligands and binding sites; free version has limits	<a href="http://tinyurl.com/relibase/">http://tinyurl.com/relibase/</a>
RSCB PDB <sup>5*</sup>	Free	US branch of wwPDB; has wide range of services	<a href="http://www.pdb.org/">http://www.pdb.org/</a>
PMP <sup>10</sup>	Free	Consolidated portal for homology-modeled structures	<a href="http://tinyurl.com/ThePMP/">http://tinyurl.com/ThePMP/</a>
Proteopedia <sup>94</sup>	Free	Community annotation of structures	<a href="http://www.proteopedia.org/">http://www.proteopedia.org/</a>
SRS 3D <sup>7</sup>	Free	Finds related structures for a sequence; displays sequence features	<a href="http://SRS3D.org/">http://SRS3D.org/</a>
Swiss-Model <sup>11</sup>	Free	Finds related structures for a sequence	<a href="http://swissmodel.expasy.org/">http://swissmodel.expasy.org/</a>
TraceSuite II	Free	Maps phylogenetic information onto structures, finds functional residues	<a href="http://tinyurl.com/TraceSuite/">http://tinyurl.com/TraceSuite/</a>

doi:10.1038/nmeth.1427



# Molecular Machinery: A Tour of the Protein Data Bank

Cells build many complex molecular machines that perform the biological jobs needed for life. Some of these machines are molecular scissors that cut food into digestible pieces. Others use one these pieces to build new molecules when cells grow or tissues need to be repaired. Some molecular machines form sturdy beams that support cells, and others are motors that use energy to crawl along these beams. Some recognize attackers and mobilize defenses against infection.

Researchers around the world are studying these molecules at the atomic level. These 3D structures are freely available at the Protein Data Bank (PDB), the central storehouse of biomolecular structures. A few examples from the ~100,000 structures held in the PDB are shown here at a magnification of about 3,500,000 times, with each atom represented as a small sphere. The enormous range of molecular sizes is illustrated here from the water molecule ( $H_2O$ ) with only three atoms (shown at the left) to the ribosomal subunits with hundreds of thousands of atoms.

## Digestive Enzymes: breaking food into small nutrient molecules

1. Amylase 1mzd
2. Phospholipase 1p0e
3. Propin 3qep
4. Protease 2d9g
5. Ribonuclease 1q5a
6. Trypsin 3zjz
7. Urease 1u00
8. Ribonuclease 3ca

## Blood Plasma Proteins: transporting nutrients and defending against infection

9. Factor X 1kak
10. Fibrin 1mij
11. Fibrin 1mij\_2bf
12. Serum Albumin 1efi

## Viruses and Antibodies: engaging in constant battle in the bloodstream

13. Antibody 1g4
14. RSVnef 4tfe

## Hormones: carrying molecular messages through blood

15. Calcitonin 1gh
16. Insulin 1di
17. Epidemic Growth Factor 1eg

## Channels, Pumps and Receptors: getting back and forth across the membrane

18. Ras Protein 3q2
19. Beta2-Adrenergic Receptor/Ca Protein 3nd
20. Glutamate Receptor 1m0
21. Epidermal Growth Factor Receptor 1tew
22. Potassium Channel 2m6
23. Phosphotransferase 4m2
24. Potassium Channel 3lu
25. Calcium Channel 1et
26. Chlorophyll ph

## Photosynthesis: harvesting energy from the sun

27. Photosystem II 1sq
28. Light-Harvesting Complex 1rxt
29. Photosynthetic Water Oxidation Center 1prc

Scale:  
1nm = 10<sup>-9</sup> meters  
1nm (nanometer) = 10<sup>-10</sup> millimeters

Extracellular Proteins

Intracellular Proteins: Cytosol

Intracellular Proteins: Cytosol

Intracellular Proteins: Nucleus

## Energy Production: powering the processes of the cell

30. Cytochrome c Oxidase (Complex III) 1eo
31. Cytochrome c1 1qcy
32. Cytochrome bc1 1bgy
33. Thermosome 1qy
34. NADH:Quinone Oxidoreductase (Complex I) 1nko
35. ATP Synthase 1e79
36. Myoglobin 1mbd
37. Hemoglobin 4tba

## Storage: containing nutrients for consumption

38. Ferritin 1hs

## Enzymes: cutting and joining the molecules of life

39. Fatty Acid Synthase 2ab2
40. RuBisCo: Ribulose Bisphosphate Carboxylase/Oxygenase 1rbcL
41. Green Fluorescent Protein 1gfp
42. Glutamine synthetase 1gq
43. Glutamine Synthetase 2g5
44. Alcohol Dehydrogenase 2gq
45. Phosphoglycerate Kinase 1tbf
46. Nitrogenase 1nif
47. Leucine Aminopeptidase 1lup
48. Lysozyme 1lyz
49. Catalase 1typ
50. Thymidylate Synthase 2hc
51. Trypsin Synthase 2hc
52. Aspartate-Glutamate-4t1

## Infrastructure: supporting and moving cells

53. Actin 1mbq
54. Myosin 1mkb
55. Intermediate Filament 1af
56. Collagen 1bbx
57. (far left)

## Protein Synthesis: building new molecular machines

58. Transfer RNA 4tqa
59. tRNA:RNA Synthetase 1gpa
60. tRNA:RNA Synthetase 1t6
61. tRNA:RNA Synthetase 1t6
62. tRNA:RNA Synthetase 1t6
63. Aspartate tRNA Synthetase 1ay
64. Ribosome 30s 1g6
65. Ribosome 50s 1g6
66. Ribosome 40S 1g6
67. elongation Factor G 1dr
68. elongation Factor Ts 1ts
69. ribosomal S6 protein 1t6
70. Chaperonin GroEL/ES 1aon
71. Prion Protein 2qpl
72. Prion Protein 2qpl
73. Prion Protein 2qpl
74. Prion Protein 2qpl
75. Prion Protein 2qpl
76. Prion Protein 2qpl
77. Prion Protein 2qpl
78. Prion Protein 2qpl
79. Prion Protein 2qpl
80. Prion Protein 2qpl
81. Prion Protein 2qpl
82. Prion Protein 2qpl
83. Ubiquitin 1ubq

## DNA: storing and reading genetic information

84. DNA 1tna
85. Restriction Endonuclease 1k6
86. DNA Polymerase 1t2
87. Topoisomerase 1t4k
88. Repressor 1tb 1tfa
89. Catalytic Core Activator 1tta
90. tRNA Binding Protein 1t6
91. DNA Helicase 4tp
92. DNA Helicase 4tp
93. DNA Polymerase 1t4
94. DNA Polymerase 1t4
95. HU Protein 1p51
96. Single-stranded DNA-binding Protein 3dsu

CC-BY-NC-ND David S. Goodsell and the RCSB PDB

PDB-101: Educational Resources. "Molecular Machinery: A Tour of the Protein Data Bank (2014)"  
<https://cdn.rcsb.org/pdb101/molecular-machinery/>

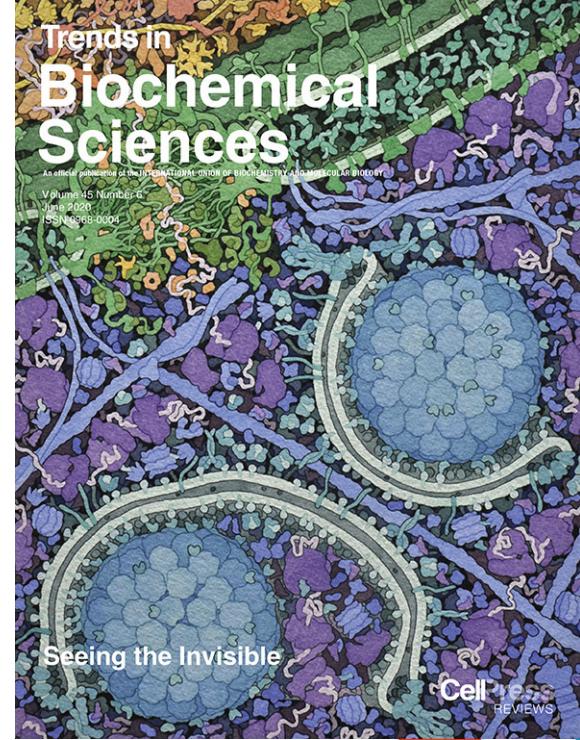
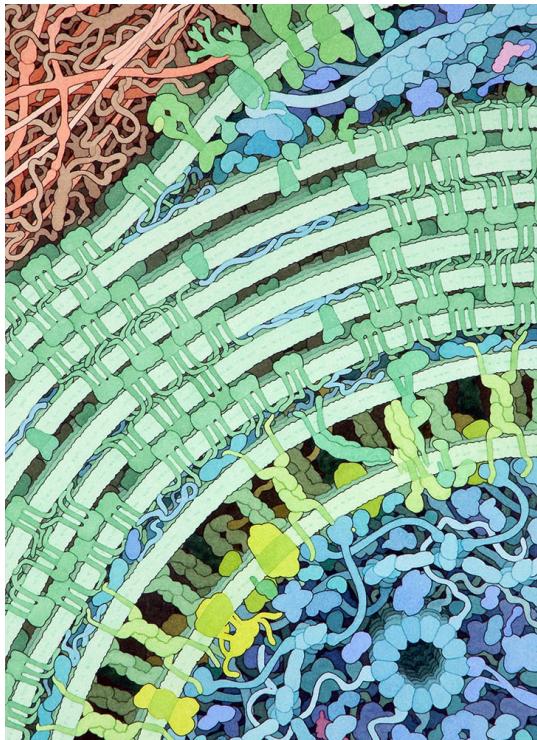
# David Goodsell



The coronavirus painting has been getting some press: Washington Post, New York Times, Forbes...  
<https://ccsb.scripps.edu/goodsell/>



# David Goodsell



<https://ccsb.scripps.edu/goodsell/>

[https://youtu.be/uHeTQLNFTgU?si=LSr5jffr5SZvKOj\\_](https://youtu.be/uHeTQLNFTgU?si=LSr5jffr5SZvKOj_)

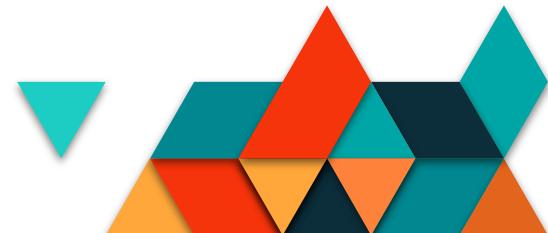
# Most Detailed Visualization of a Cell Ever Created



This 3D model of a eukaryotic cell was created using X-ray, nuclear magnetic resonance (NMR), & cryo-electron microscopy datasets.

It's an attempt to visualize the many pathways involved in cellular processes (i.e. signal transduction, protein synthesis, endocytosis, vesicular transport, cell-cell adhesion, apoptosis) as well as the great complexity & beauty of the cell's molecular machinery.

Cellular landscape cross-section through a eukaryotic cell, by Evan Ingersoll & Gael McGill  
[https://www.digizyme.com/cst\\_landscapes.html](https://www.digizyme.com/cst_landscapes.html)



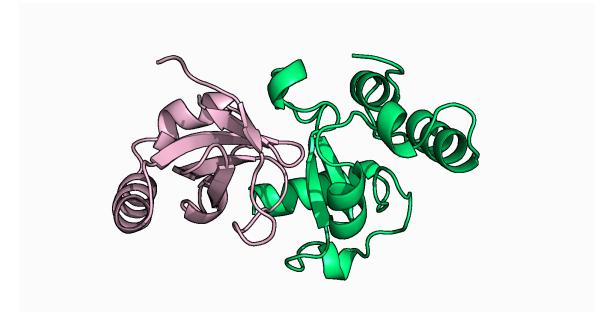
# Type of Files

---

PDB                    } Macromolecules  
PDBQ(T)                (Proteins/Nucleic Acids)

MOL2                    }

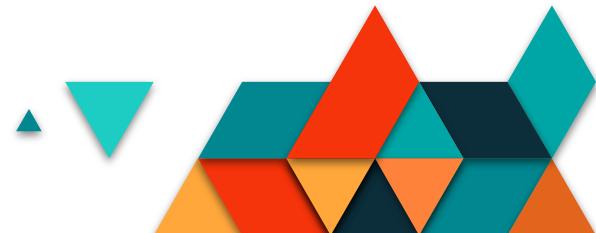
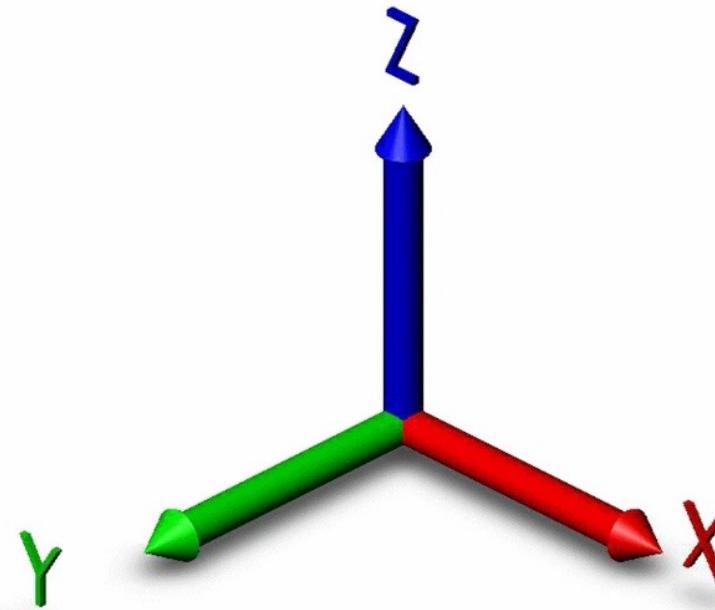
SDF                    } Macromolecules (Small  
SMILES                Molecules/Drugs)



# Type of Files

## Coordinates:

- Absolute
- Relative



# PDB Files

ATOM	1	N	LYS	A	1	-14.294	-3.055	2.337	1.00	2.14	N
ATOM	2	CA	LYS	A	1	-13.199	-3.713	1.562	1.00	1.60	C
ATOM	3	C	LYS	A	1	-12.868	-2.889	0.312	1.00	1.05	C
ATOM	4	O	LYS	A	1	-13.563	-2.946	-0.688	1.00	1.74	O
ATOM	5	CB	LYS	A	1	-13.740	-5.096	1.178	1.00	2.47	C
ATOM	6	CG	LYS	A	1	-13.597	-6.047	2.369	1.00	3.16	C
ATOM	7	CD	LYS	A	1	-13.360	-7.474	1.866	1.00	4.03	C
ATOM	8	CE	LYS	A	1	-14.074	-8.465	2.790	1.00	4.82	C
ATOM	9	NZ	LYS	A	1	-13.969	-9.785	2.107	1.00	5.62	N
ATOM	10	H1	LYS	A	1	-14.563	-3.656	3.141	1.00	2.56	H
ATOM	11	H2	LYS	A	1	-15.119	-2.909	1.719	1.00	2.60	H
ATOM	12	H3	LYS	A	1	-13.961	-2.137	2.691	1.00	2.50	H
ATOM	13	HA	LYS	A	1	-12.319	-3.823	2.179	1.00	1.96	H
ATOM	14	HB2	LYS	A	1	-14.783	-5.012	0.905	1.00	2.99	H
ATOM	15	HB3	LYS	A	1	-13.178	-5.482	0.342	1.00	2.86	H
ATOM	16	HG2	LYS	A	1	-12.761	-5.736	2.979	1.00	3.36	H
ATOM	17	HG3	LYS	A	1	-14.501	-6.022	2.959	1.00	3.51	H
ATOM	18	HD2	LYS	A	1	-13.747	-7.572	0.861	1.00	4.31	H
ATOM	19	HD3	LYS	A	1	-12.301	-7.683	1.866	1.00	4.31	H
ATOM	20	HE2	LYS	A	1	-13.583	-8.498	3.754	1.00	4.89	H
ATOM	21	HE3	LYS	A	1	-15.110	-8.191	2.905	1.00	5.17	H
ATOM	22	HZ1	LYS	A	1	-14.503	-10.496	2.644	1.00	6.13	H
ATOM	23	HZ2	LYS	A	1	-12.969	-10.069	2.053	1.00	5.71	H
ATOM	24	HZ3	LYS	A	1	-14.362	-9.713	1.147	1.00	5.90	H
ATOM	25	N	TRP	A	2	-11.809	-2.120	0.370	1.00	0.67	N
ATOM	26	CA	TRP	A	2	-11.408	-1.281	-0.798	1.00	0.57	C
ATOM	27	C	TRP	A	2	-9.877	-1.179	-0.857	1.00	0.43	C
ATOM	28	O	TRP	A	2	-9.212	-1.099	0.161	1.00	0.49	O
ATOM	29	CB	TRP	A	2	-12.047	0.093	-0.535	1.00	1.16	C



# PDB Files

ATOM records- Common AA and Nucleotides only

```
ATOM  1      N   ILE J 11    5.804 123.968 147.434  1.00 94.01  N
ATOM  2      CA  ILE J 11    5.791 123.831 145.944  1.00 93.94  C
ATOM  3      C   ILE J 11    7.198 123.695 145.333  1.00 92.32  C
ATOM  4      O   ILE J 11    8.169 124.255 145.843  1.00 93.52  O
...
TER      6327    ASP J 431
HETATM 6328  O  HOH J2001  4.852 121.472 146.292  1.00 50.45  O
HETATM 6329  H1 HOH J2001  4.622 120.611 146.642  1.00  0.00  H
...
CONECT 6329 6328
CONECT 6330 6328
...
END
```



# PDB Files

HETATM records- All other atoms

CONECT records- bonds between HETATMs

-Don't include bond order so not for general use

```
ATOM  1      N   ILE J 11      5.804 123.968 147.434  1.00 94.01  N
ATOM  2      CA  ILE J 11      5.791 123.831 145.944  1.00 93.94  C
ATOM  3      C   ILE J 11      7.198 123.695 145.333  1.00 92.32  C
ATOM  4      O   ILE J 11      8.169 124.255 145.843  1.00 93.52  O
...
TER      6327    ASP J 431
HETATM 6328  O  HOH J2001  4.852 121.472 146.292  1.00 50.45  O
HETATM 6329  H1 HOH J2001  4.622 120.611 146.642  1.00  0.00  H
...
CONECT 6329 6328
CONECT 6330 6328
...
END
```



# mol2 Files

```
@<TRIPOS>MOLECULE
3ZWZ.pdb
2892 2732 564 0 0
PROTEIN
NO_CHARGES

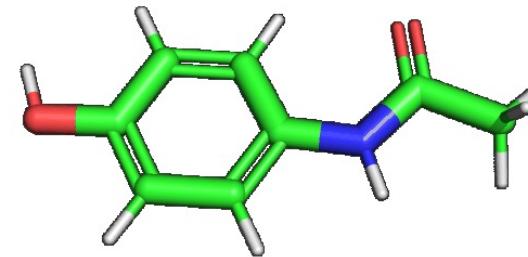
@<TRIPOS>ATOM
  1 N      -15.6500  14.3770  5.0450 N.4      1 ASN   0.0000
  2 CA     -15.2850  13.0110  5.5660 C.3      1 ASN   0.0000
  3 C      -15.8880  12.7820  6.9380 C.2      1 ASN   0.0000
...
@<TRIPOS>BOND
  1 328 1568 1
  2 866 1109 2      (Includes bond order so can be used for ligands)
...
@<TRIPOS>SUBSTRUCTURE
  1 ASN   2 RESIDUE      4 A   ASN   1 ROOT
  2 PRO   10 RESIDUE     4 A   PRO   2
```



# SMILES

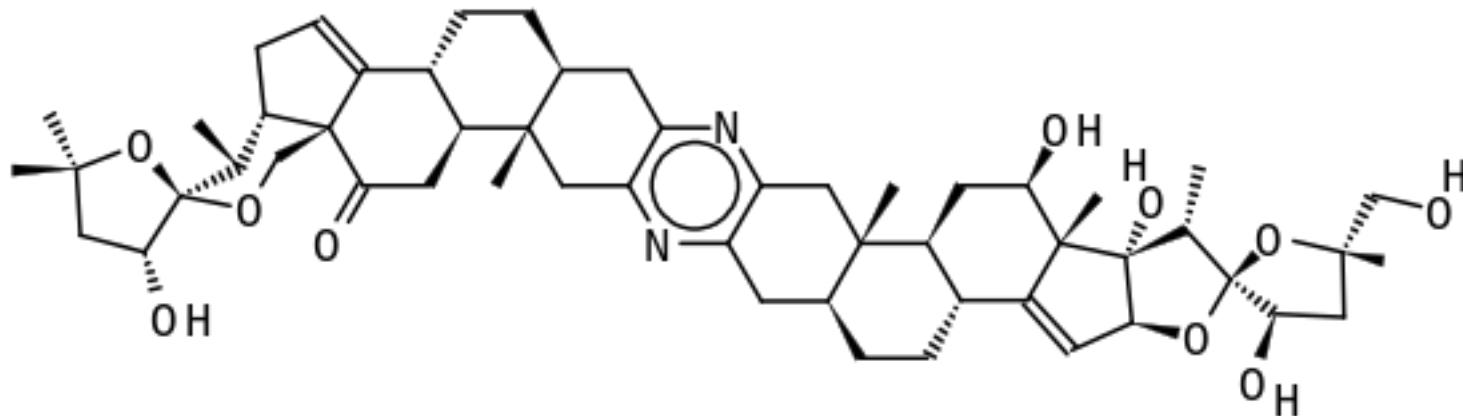
- Simplified molecular-input line-entry system
- A notation that allows users to describe the structure of chemical species using short ASCII strings.

CC(=O)NC1=CC=C(C=C1)O



# SMILES

- Simplified molecular-input line-entry system



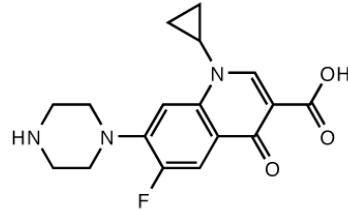
Ex: Cephalostatine

```
CC(C)(O1)C[C@@H](O)[C@@]1(O2)[C@@H](C)[C@@H]3CC=C4[C@]3(C2)C(=O)
C[C@H]5[C@H]4CC[C@@H](C6)[C@]5(C)Cc(n7)c6nc(C[C@@]89(C))c7C[C@@H]8
CC[C@@H]%10[C@@H]9C[C@@H](O)[C@@]11(C)C%10=C[C@H](O%12)[C@]
%11(O)[C@H](C)[C@]12(O%13)[C@H](O)C[C@@]13(C)CO
```

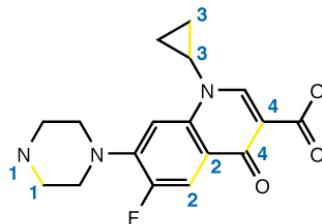


# SMILES

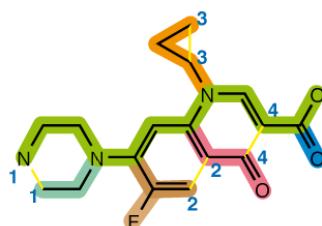
A



B



C

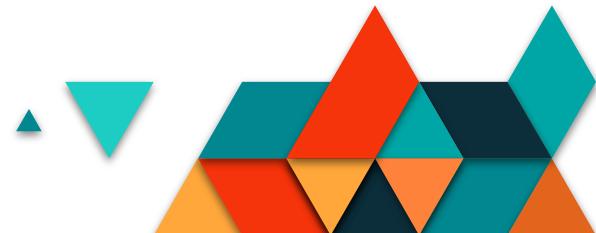


D

N1CCN(CC1)C(C(F)=C2)=CC(=C2C4=O)N(C3CC3)C=C4C(=O)O

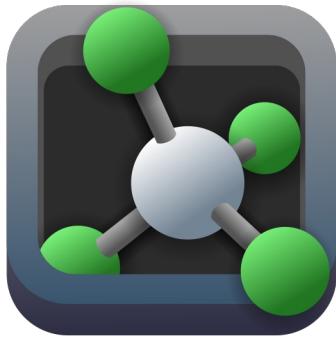
## Generation of SMILES:

Open the rings and write them as branches of the main chain.



# Molecular Viewers

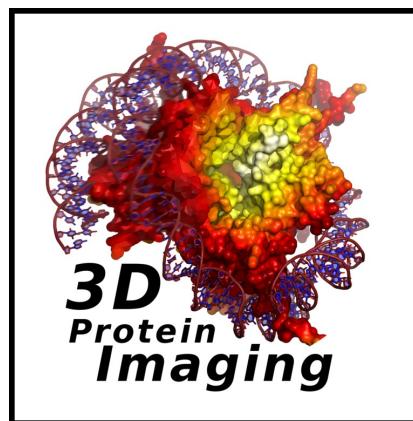
---



Pymol



ucsf  
Chimera

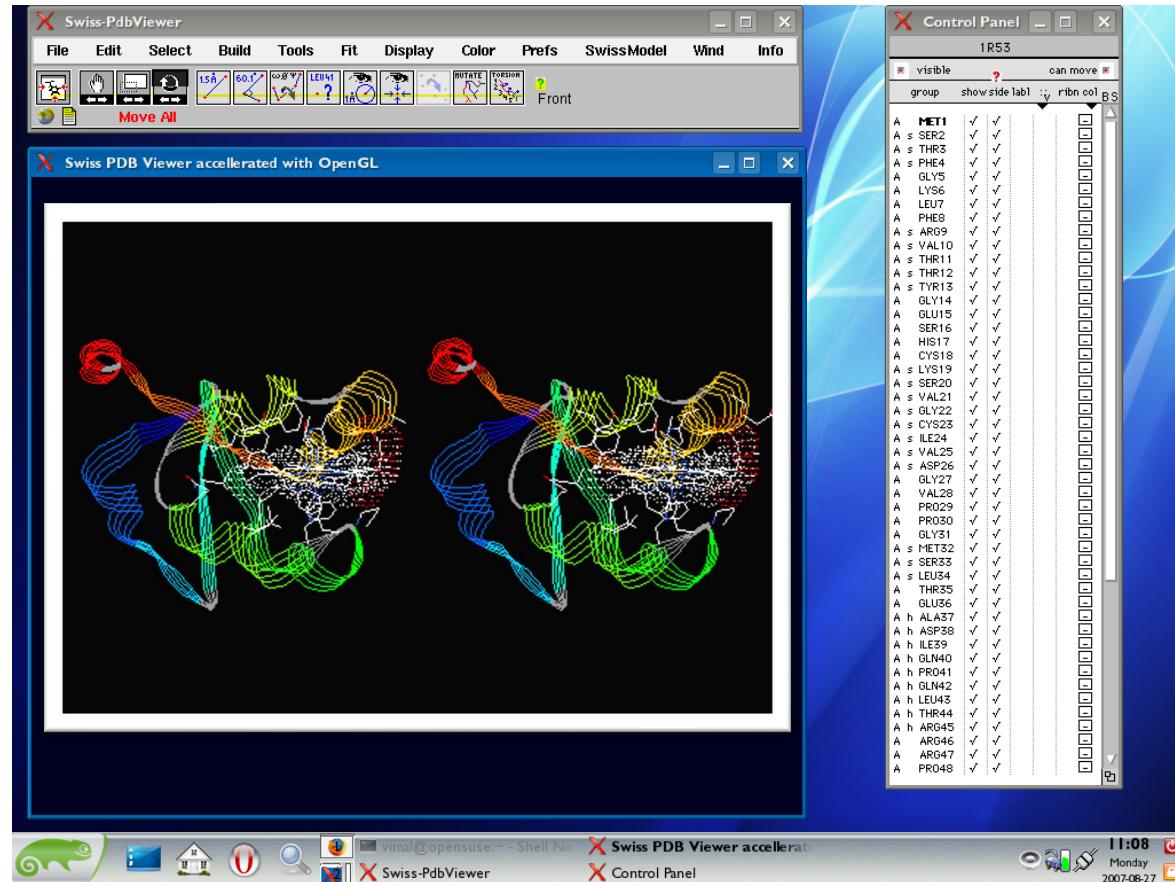


3Dmol.js



**VMD**  
Visual Molecular Dynamics

# SPDBV



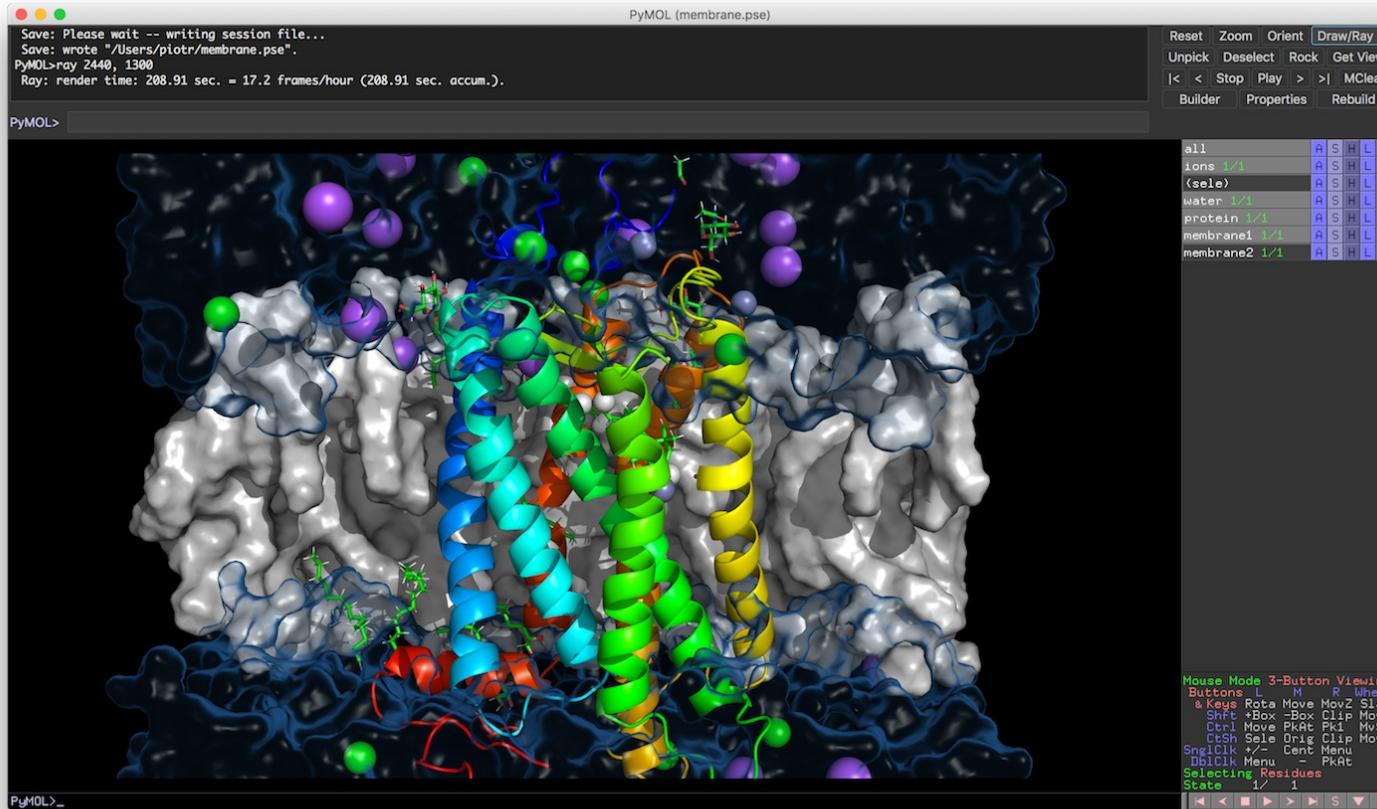
vimal@opensuse:~ - Shell No. 11:08  
X Swiss PdbViewer accelerated  
X Control Panel

Monday  
2007-08-27

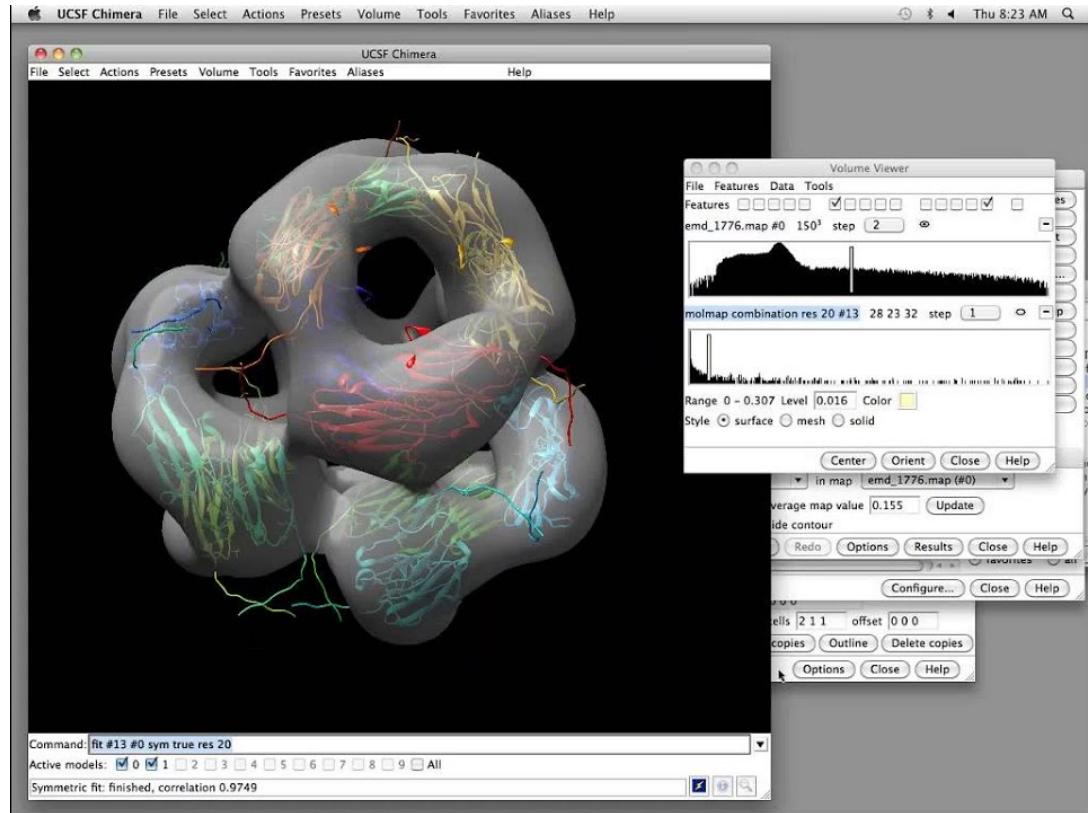
<https://spdbv.unil.ch/>



# pyMOL

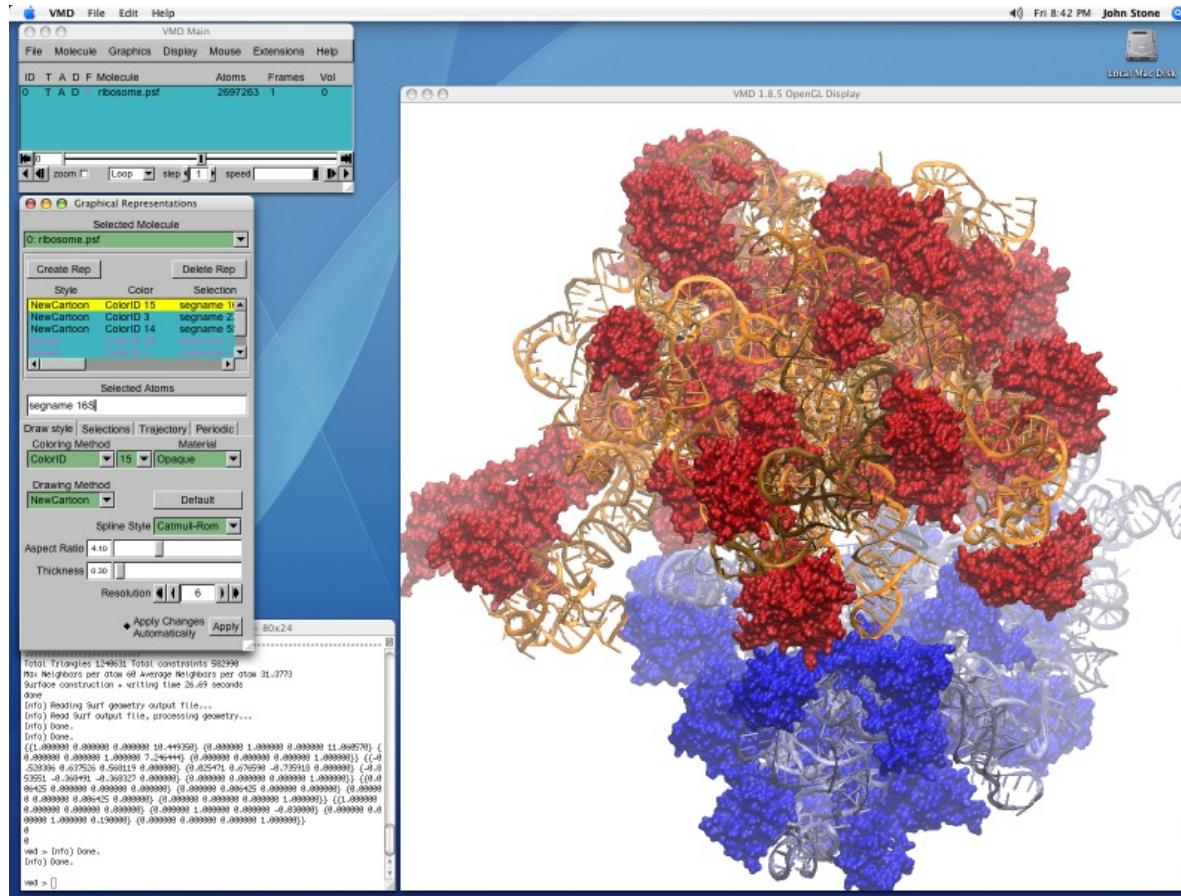


# UCSF Chimera



<https://www.cgl.ucsf.edu/chimera/>

VMD

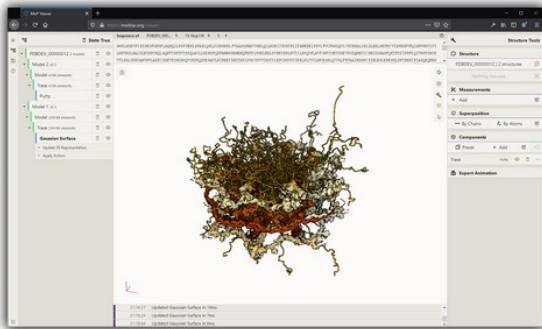


<https://www.ks.uiuc.edu/Research/vmd/>

# Online Molecular Viewers



Mol\* ([/molstar/](https://molstar.org/)) is a modern web-based open-source toolkit for visualisation and analysis of large-scale molecular data



[Open Mol\\* Viewer](#)

[Viewer Documentation](#)

[Issues & Feedback](#)

High-performance graphics and data handling of the Mol\* Viewer allow users to simultaneously visualise up to hundreds of (superimposed) protein structures, play molecular dynamics trajectories, render cell-level models at atomic detail with tens of millions of atoms, or display huge models obtained by I/HM such as the Nuclear Pore Complex.

<https://molstar.org/>



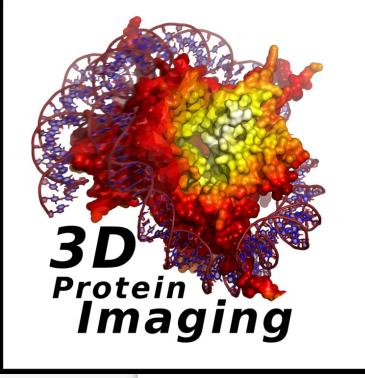
# Online Molecular Viewers

Protein Imager  [Login](#) [Register](#)

Visual selection  
Pick on screen to select **Disabled**

Structure hierarchy ?  
STRUCTURE 1

Advanced selections  
By Entity   By Proximity  
By Range   By Property



3D Protein Imaging

Structures  
Change structure 

Structures superimposition

Current structure  
STRUCTURE 1  
FILE NAME: NOT FOUND  
TITLE: STRUCTURAL CHARACTERIZATION OF H3K56Q NUCLEOSOMES AND NUCLEOSOMAL ARRAYS

Assembly  
DEFAULT

Selections ?  
x Restore default selections  
+ New selection

Entity	Count
Protein str. 1	6007
Nucleic str. 1	5980
Ligands str. 1	0
Water str. 1	23

 Log history Sequence viewer Viewing options Animation controls Distances Membrane

<https://3dproteinimaging.com/protein-imager/>

# Online Molecular Viewers

[About](#)[Launch](#)[Help](#)[Gallery](#)[Contact](#)

## 3-dimensional structure Representation Sharing

### Welcome to 3dRS



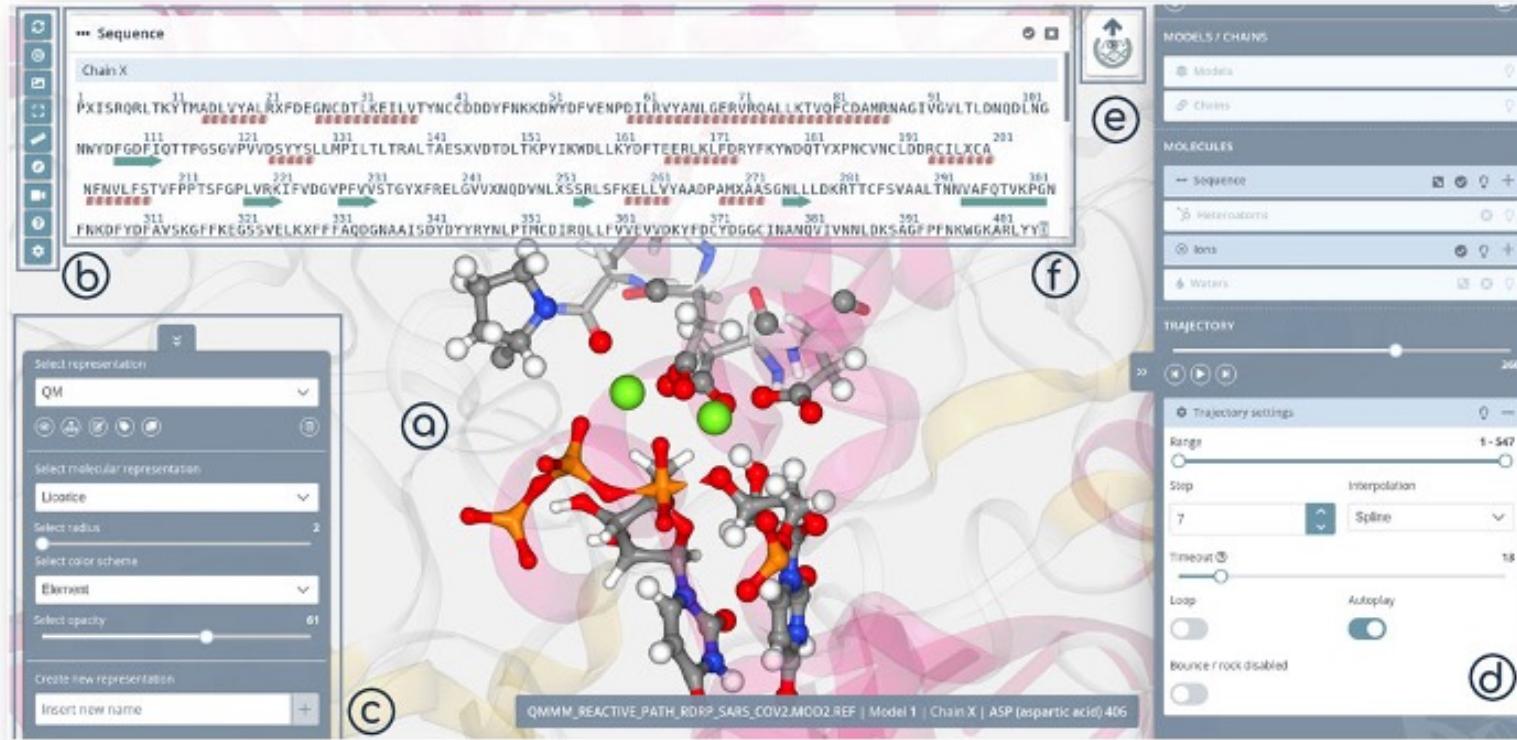
The **3-dimensional structure Representation Sharing (3dRS)** web application has been built with the aim of **sharing visualizations of 3D biological structures** through the web. In these visualizations, users will be able to draw several representations with different selections of the structure(s) previously **uploaded to the application**.

Our **philosophy for this project** is to make it accessible to everybody, so there is no private area and once a project is shared **everybody with the link can access it** with no restrictions.

<https://mmb.irbbarcelona.org/3dRS/>



# Online Molecular Viewers



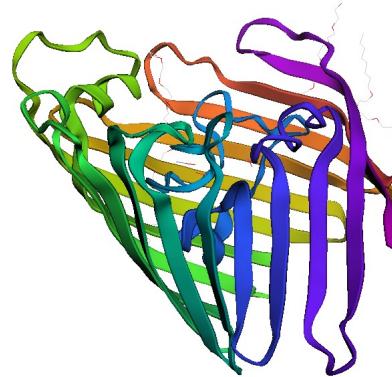
<https://mmb.irbbarcelona.org/3dRS/>

# Online Molecular Viewers

## 3Dmol.js

View Embed Teach Jupyter Develop

*A modern, object-oriented JavaScript library for visualizing molecular data*



## py3Dmol

A simple [IPython/Jupyter](#) widget to embed an interactive [3Dmol.js](#) viewer in a notebook.

The widget is completely static, which means the viewer doesn't need a running IPython kernel to be useful and web pages and presentations generated from the notebook will work as expected. However, this also means there is only one-way communication between the notebook and the viewer.

<https://3dmol.org/>



# Virtual Reality (VR)

The Future of Molecular Design

Global real-time collaboration using Virtual Reality from general chemistry to pharmaceutical drug discovery.

Play Video ▶

Schedule a Demo

MARA Plugins Plugins Resources Login Demo Download

Chemical Properties

loading...

Molecule 395.503MW 2.248logP 65.040TRs

Docking - 2024 (Thrombin)

Docking - Thrombin

Docking - 2023

Docking - 2022

Chemical structure: C=CC1=C(C=C1)N2COC2=O

## Most Effective Tool for Drug Design Decision Making

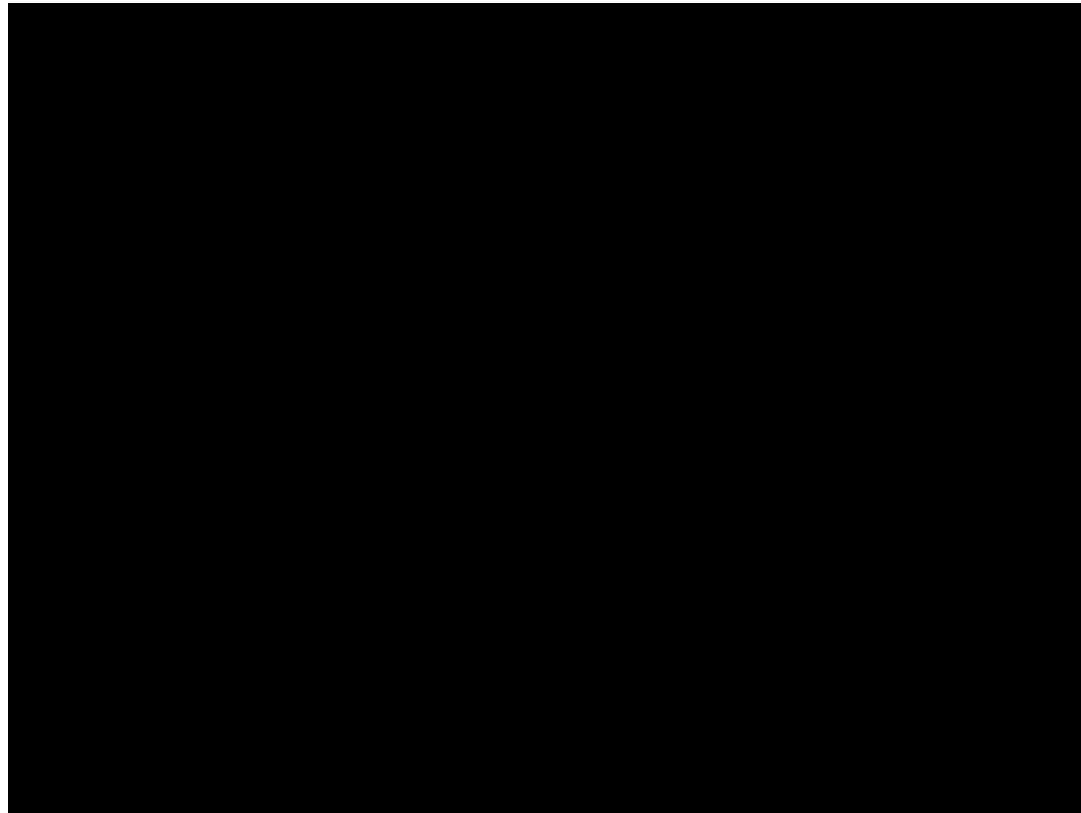
Integrate with tools, workflows, and team members all over the world

<https://nanome.ai/>

# Virtual Reality (VR)



# 3D Printing

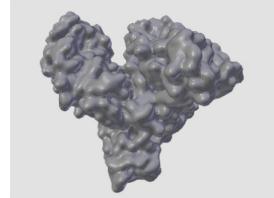


Da Veiga Beltrame, E., Tyrwhitt-Drake, J., Roy, I., Shalaby, R., Suckale, J., & Pomeranz Krummel, D. (2017). 3D Printing of Biomolecular Models for Research and Pedagogy. *Journal of visualized experiments : JoVE*, (121), 55427. <https://doi.org/10.3791/55427>



# 3D Printing

## 3D Model Information



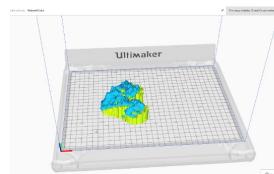
PDB structure used to generate the model file: [1e7i](#)

Model generated with: Molecular Maya/Autodesk Maya

Model physical size (in mm): 90 x 52 x 90

[Download 3D Print File \(.stl\)](#)

## Sample print



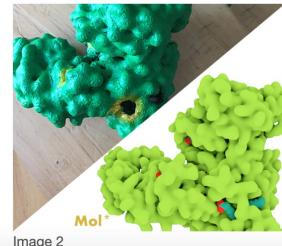
**Printed on:** Ultimaker S3. The image on the left shows the support system generated by the printer in the printer interface. The image on the right shows the printed model with support system removed. We recommend keeping the model in the water bath for a couple of days to fully dissolve the support material inside the hydrophobic tunnels.

**Model material:** PLA

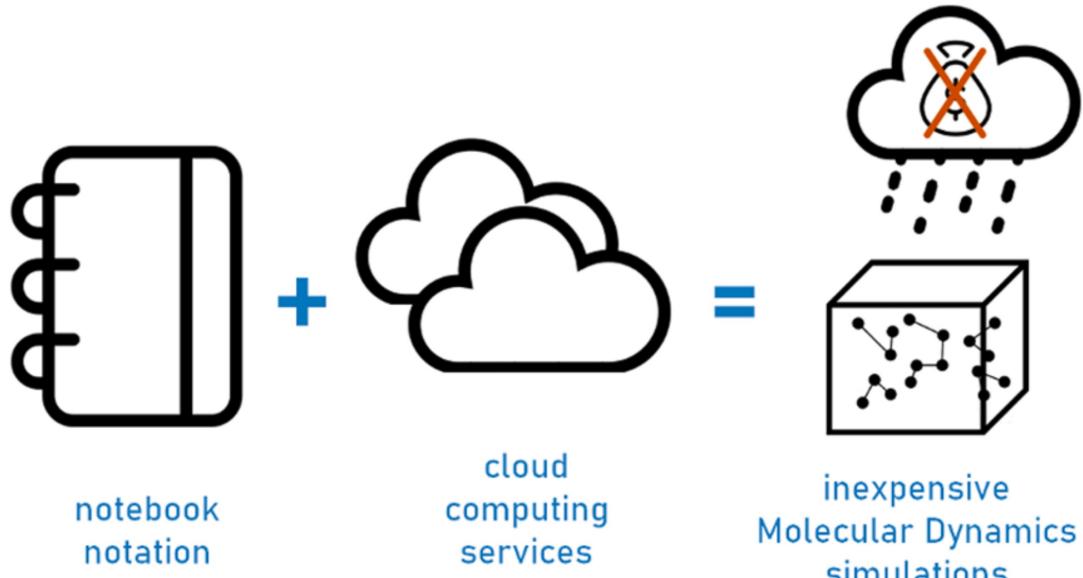
**Support material:** PVA (water soluble)

**Output scale:** 100%

## 3D Print and Structural Features of Alpha-amylase



# Making it Rain



<https://pablo-arantes.github.io/making-it-rain/>



# Notebook - Macromolecular Visualization

Hello there!

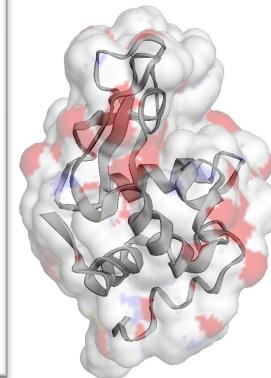
This is a Jupyter notebook to visualization of macromolecular systems using py3dmol. This notebook is based on "***Making it rain: Cloud-based molecular simulations for everyone***" ([link here](#)). This notebook is part of BIEN 165 class of bioengineering course at University of California, Riverside.

Notebook created by [Pablo R. Arantes](#)

The main goal of this notebook is to demonstrate the steps to visualize a macromolecular systems in a cheap and yet feasible fashion.

## Acknowledgments

- A Making-it-rain team, Pablo R. Arantes ([@pablitoarantes](#)), Marcelo D. Polôto ([@mdpoloto](#)), Conrado Pedebos ([@ConradoPedebos](#)) and Rodrigo Ligabue-Braun ([@ligabue\\_braun](#)).
- Also, credit to [David Koes](#) for his awesome [py3Dmol](#) plugin.
- For related notebooks see: [Making-it-rain](#)



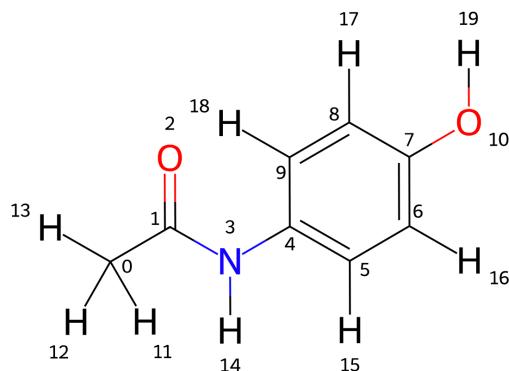
SCAN ME

<https://github.com/pablo-arantes/BIEN165>



# Notebook - Micromolecular Visualization

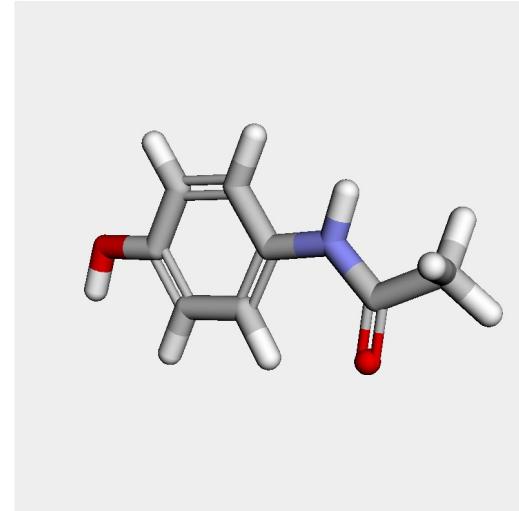
Smiles: CC(=O)NC1=CC=C(C=C1)O



> Show 3D structure of your molecule:

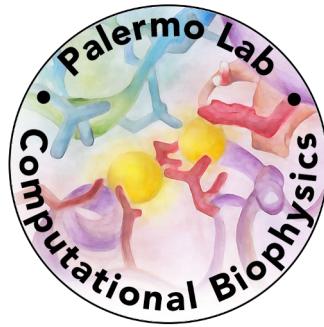


Show code



<https://github.com/pablo-arantes/BIEN165>





Department of Bioengineering  
University of California Riverside  
223 Materials Science & Engineering  
900 University Ave. | Riverside, CA 92521

<https://palermolab.com/>



website

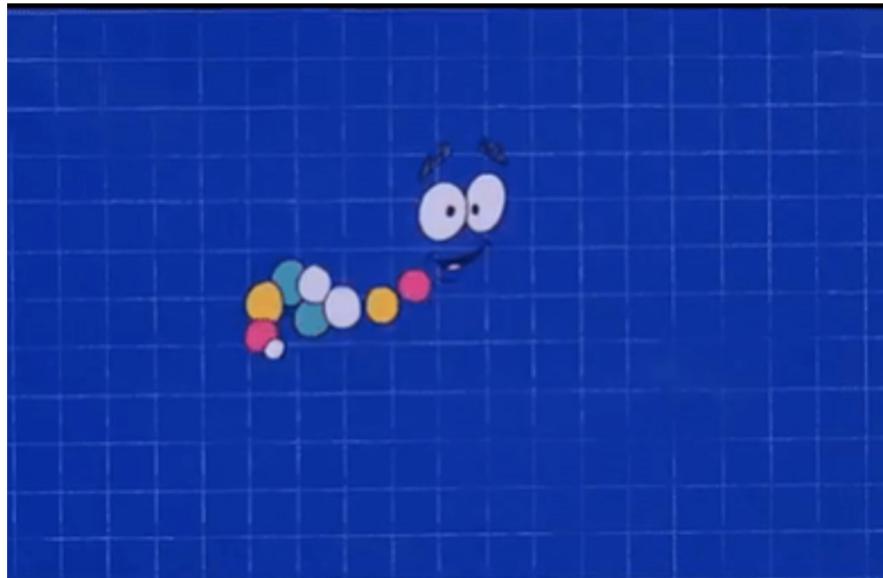


SCAN ME

pablitoarantes@gmail.com

pabloa@ucr.edu

<https://pablo-arantes.github.io>



twitter



SCAN ME



# Obrigado (Thank you)! ☕

