SBGrid

Using SBGrid @ Biochem v1.1.0

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Foreword

The SBGrid Consortium software collection is available within the Biochemistry department when connected to the network properly. This document is meant to inform you about SBGrid and how to access it from your computer. However, note that SBGrid software only run on Macintosh with Intel processors as well as Intel Linux 32 or 64 bit operating systems.

While many of the software are available for individual download from the original authors, the advantage of SBGrid is to offer the software already installed, updated and ready to use.

The SBGrid team has a YouTube channel that offers training on specific software included within the SBGrid panel of available software.

The “SBGrid Consortium” channel is at **youtube.com/user/SBGridTV**

About SBGrid

The SBGrid Consortium web site **sbgrid.org** describes in detail the history of its inception in the year 2000 at the Harvard University structural biology laboratories of Stephen Harrison and the Don Wiley by structural biologist Piotr Sliz.

SBGrid's NIH-compliant Service Center supports SBGrid operations and provides members with access to the following services and resources:

Software Maintenance: The SBGrid Center manages the support cycles of 250+ scientific applications.

1. Applications categories

The SBGRid Consortium web site offers the following categories to list applications on the left hand side menu under "**Supported Applications**" but the web page offers the option to "**Filter by Category**" with a more choices:

- All Software
- X-ray Crystallography
- NMR Methods
- Structure Analysis
- 2D Crystallography
- Electron Microscopy
- Structure Visualization
- Nucleic Acids
- Computational Chemistry
- SAXS (small-angle scattering)
- Tomography

- Bioinformatics
- Utilities

For a list of applications and a short description refer to the Appendix page 18 or go the the SBGrid web site for the most up-to-date list: **https://sbgrid.org/**

Set-Up

All software is run on your local computer when connected to a remote server. The only requirement is to be connected to the Biochemistry network either by being present within the Biochemistry network system on Campus, or by using a VPN connection to the network.

Requirements:

- Biochemistry user account. If you need to have your account set-up visit the IT department on the 4th floor of the **HF DeLuca Biochemistry Laboratories Building**. See General IT Questions at **https://biochem.wisc.edu/intranet/it/general-questions**
- Administrative privileges to install software on the computer

1. SBGrid Installation

In this section we will fetch a small (300 Kb) installer from the Biochemistry Department Intranet.

This installation procedure only needs to be done one time on the computer(s) you want to use.

In specific cases it would be possible to install the complete SBGrid within a laptop (*e.g.* to travel to a conference) but that installation would require 250Gb of free drive space and should be done with the help of the IT department.

SBGrid only runs on Macintosh and Linux systems. For a Microsoft Windows operating system the installation of a virtual Linux could allow access.

1.1. Fetch and install SBGrid

Using the web browser of your choice connect to the Biochemistry Intranet **https://biochem.wisc.edu/**

- **Click** INTRANET in the top tab list and select **IT**

- On the next page, on the right column click "**Available Software**"
- Within the software list in the page **locate and click on**:
  SBGrid (*Biochem username/password required*)

You will be required to login with your **UW NetID**. and presented with a very simple page from which you can download the software:

The Biochemistry Department has a special license arrangement for SBGrid.

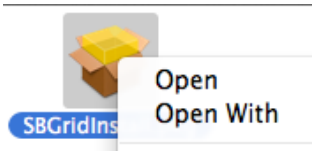
This software is licensed for regular use by **Butcher, Fox, Henzler-Wildman, Holden, Markley, Mitchell, Phillips** and **Rayment** Labs. All other users may use the software for occasional use only. If you use the software regularly please contact IT to have your lab added.

Access to this software is licensed for **ACADEMIC USE ONLY**, this software may not be used in any for-profit work!

For detailed information about SBGrid and a list of the software it offers, please visit the SBGrid website at **https://sbgrid.org**.

Attachment	Size
sbgridmacinstaller.dmg	229.95 KB

- **Click on sbgridmacinstaller.dmg** download the installer file within your default download directory Alternatively right-click (or control-click) and choose where you want to save the file.
- This is a "disk image." When clicked or double-clicked a virtual disk volume icon will appear on the desktop.
- **Open the virtual disk** and **double click** on the one file within named `SBGridInstall.pkg`



- If your computer complains that it cannot open the file "*because it is from an unidentified developer*" use a control-click or **right-click** instead and **choose Open**
- A new warning security window will appear: **click "Open"** (the default option is "Cancel" if you just press return.)
- Finally you will be required to validate the installation with your *administrator password*.

Once the installation is successful a new “app” named “SBGrid” will be located within the Applications folder. Its real name is SBGrid.app but that depends on your folder view settings.

SBGrid can now be used on this computer provided the proper server connections are active as detailed in the next section.

1.2. Connect to *Groups* server

The SBGrid software package is very large and stored used on a network connection to a drive that contains all of the packages. To use the software it is necessary to connect to the server.

On a Macintosh follow these instructions to connect to the *Groups* drive:

- **Click anywhere** on the desktop to see the Finder menu at the top of the screen
- In the Finder menu use **Go > Connect to Server…**
- In the server address type: **`afp://file.biochem.wisc.edu`**
- Click “Connect”
- Enter your *username* and *password* (Biochem. *or* NetID)
- In the volume list **select Groups** and any other volume you want to see.
- Depending on your Finder settings you will see a new icon on the desktop named Groups with a shared icon look. If you don’t see an icon it OK.

1.2.1. VPN connection

If connecting outside the Biochemistry department it will be necessary to connect via a Virtual Private Network (VPN) to mimic local presence.

Please refer to the following resources to install and activate VPN:

General University description:

https://it.wisc.edu/services/wiscvpn/

Biochemistry Department Intranet instructions:

https://biochem.wisc.edu/intranet/it/remote-access

1.3. Activating SBGrid

Every time you want to use SBGrid you will need to locate and double click on the *SBGrid.app* shield icon and be connected to the *Groups* network volume.

The activation will open a new Terminal from which all software need to be started, even if they have a graphical interface.

- Step 1: **double click** the *SBGrid.app* shield icon

- Step 2: a new terminal window will open with a statement to which you need to answer affirmatively with a capital **Y**:

```
*******************************************************************************
 UW-Madison Biochemistry has licensed SBGrid. This software is licensed for
 regular use by Butcher, Fox, Holden, Markley, Mitchell, Phillips and Rayment
 Labs. All other users may use the software for occasional use only. If you
 use the software regularly please contact IT to have your lab added.

 Access to this software is licensed for ACADEMIC USE ONLY, this software may
 not be used in any for-profit work!

 You may silence this message by entering 'YY' at the prompt.
*******************************************************************************

 I agree this software will only be used for academic purposes! (enter 'Y')
>
```

- After answering "**Y**" a start-up screen will confirm activation for this session:

```
>Y

*******************************************************************************
 Starting SBGrid
*******************************************************************************

                  Software Support by SBGrid (www.sbgrid.org)
*******************************************************************************
 Your use of the applications contained in the /programs  directory constitutes
 acceptance of  the terms of the SBGrid License Agreement included  in the file
 /programs/share/LICENSE.  The applications  distributed by SBGrid are licensed
 exclusively to member laboratories of the SBGrid Consortium.
*******************************************************************************
 SBGrid was developed with support from its members, Harvard Medical School,
 HHMI, and NSF. If use of SBGrid compiled software was an important element
 in your publication, please include the following reference in your work:

 Software used in the project was installed and configured by SBGrid.
 cite: eLife 2013;2:e01456, Collaboration gets the most out of software.
*******************************************************************************
 SBGrid installation last updated: 2016-06-07
 Please submit bug reports and help requests to:       <bugs@sbgrid.org>  or
                                                       <http://sbgrid.org/bugs>
*******************************************************************************
```

Note: these text screens above are specific to the Biochemistry Department.

1.3.1. The $ prompt

The terminal is a plain text window that is expecting (waiting for) a command which is given at the "prompt" represented by a sign that can be `$` in many cases but could also be `#` or `%` depending on the circumstances.

See page 12 for commands to start an SBGrid program.

1.4. Troubleshooting SBGrid activation

If you get the following error screen upon activation of the SBGrid.app software:

```
*******************************************************************************
 ERROR!!!
 You are not currently connected to the Groups share on the File Server, do not
 have permissions to use SBGrid or are not the only user connected to it. You
 must have permissions and be connected to Groups for SBGrid to work properly.

 Please connect to the Group share properly and run this script again or contact
 IT to find about gaining permission to use SBGrid.
*******************************************************************************
```

To remedy this problem connect to the *Groups* server as detailed above. If the error persists, contact the IT department by *e.g.* opening a "ticket" on the job board.

1.5. Software Help

A wiki is available at **sbgrid.org/wiki/** with the following useful information:

If the problem with the software started after an update, you can configure your SBGrid environment to use an older version of the software. (**http://sbgrid.org/wiki/usage/versions**)

However, most of the wiki are for system administrators installations.

2. Using SBGrid

Using SBGrid on a computer where it has been installed requires the two steps detailed above with two additional requirements preferably in the following order:

1) Being within the Biochem network or connected via VPN
2) Being connected to the Groups network volume
3) Activating *SBGrid.app* by double-clicking on the shield icon
4) Answering "Y" at the prompt question

2.1. Starting an SBGrid program

An SBGrid software is activated by typing its name at the Terminal console, whether it is a line-command or GUI (Graphical User Interface) software. The list of software is available on the SBGrid consortium web site (**sbgrid.org**) under the "**Supported Applications**" tab on the left.

The name to type is typically the software name in lower case. However, in some cases the packages contain many multiple programs that need to be called specifically.

For example, the first software listed in the list of applications is called "**2dx**" but typing that at the console will not work because this particular software is split between 3 executable files: `2dx_image`, `2dx_logbrowser` and `2dx_merge`. In the same way the packages "**ImageMagick**" or "**EMBOSS**" are collections of many individual executable files that need to be called separately, for example `convert` to call on the image conversion program of "**ImageMagick**" or `water` to call the Smith-Waterman local alignment program from the "**EMBOSS**" package.

A table showing the list of applications for the Macintosh is presented in the Appendix 1.1 below on page 17.

Other software are simpler to start, for example the molecular graphics programs VMD, Rasmol, PyMOL and Chimera are started with the following commands in the SBGrid Terminal console after the `$` prompt:

```
$ vmd
$ rasmol
$ pymol
$ chimera
```

and the appropriate program will launch. However, it is recommended to add the ampersand (&) after the command so that the software is run in the background and you get the $ prompt back for more commands if needed.

Therefore the command should be issued as:

```
$ vmd &
```

```
$ rasmol &

$ pymol &

$ chimera &
```

Line command software will be activated in a similar way and the Terminal itself will be used to run the software.

2.2. Software versions: `sbgrid`

Many of the SBGrid software are present in 3 versions. The newest version is the one used by default when activated. To list which versions exist currently in the SBGrid installation use the `sbgrid` command to request a list for the current computer in use (here a Macintosh.) For example here are the version available for PyMOL:

```
$ sbgrid -l pymol
```

```
  Version information for: /programs/i386-mac/pymol

Default version:                    1.8.2.1
In-use version:                     1.8.2.1
Other available versions:           1.8.0.5 1.7.6.6 1.7.2.3
1.6.0.0 1.5.0.2 1.4.1-x11
Overrides use this shell variable:  PYMOL_M
```

The modifier -L for sbgrid will list software available on all platforms (Linux 32, 64 and OS X).

```
$ sbgrid -L pymol
```

```
Version information for: /programs/i386-mac/pymol

Default version:                    1.8.2.1
In-use version:                     1.8.2.1
Other available versions:           1.8.0.5 1.7.6.6 1.7.2.3
1.6.0.0 1.5.0.2 1.4.1-x11
Overrides use this shell variable:  PYMOL_M

  Version information for: /programs/i386-linux/pymol

Default version:                    1.7.2.1
Other available versions:           1.6.0.0 1.5.0.5 1.5.0.4 1.3
Overrides use this shell variable:  PYMOL_L

No program directory by that name found in /programs/powermac.
```

As shown on the listings, the default version is contained within a variable specific for the software and for the platform. To learn more about shell variable refer to a generic Unix or Linux manual.

You can print the current value of a shell variable with the `printenv` command.

For example:

```
$ printenv PYMOL_M
```

```
1.8.2.1
```

The specific suffix `_M` is appended for the Macintosh (`i386-mac`) while the suffix `_L` is used for `i386-linux` and `_X` for `x86_64-linux`.

Note: `printenv` issued alone without argument will print all know environment shell variable at once on the Terminal screen.

For more details on selecting, or disabling versions consult the SBGrid wiki at **https://sbgrid.org/wiki/usage/versions**

2.3. Version override

In some cases it may be useful to override the default version of a software.

Full details of the override method can be found on the web site: **sbgrid.org/wiki/usage/versions**

Briefly this is accomplished by modifying the `~/.sbgrid.conf` file in your home directory. It can be edited with your default editor with the command:

```
$ sbgrid-overrides -e.
```

On a Mac this will open the `~/.sbgrid.conf` file within TextEdit.

Default `~/.sbgrid.conf` file:

```
# /Users/xxx/.sbgrid.conf: override default application
#   versions for SBGrid software.
#
# One override per line in VARIABLE=value format.
Examples:
#
# To use the PHENIX nightly version on OS X Intel:
# PHENIX_M=nightly
#
# To use use an older version of CCP4 on linux:
# CCP4_X=6.2.0
#
# Add your override settings below
```

To override a version check the versions available (see above) and provide one override command per line.

For example to use on older version of PyMOL on a Mac one would enter the following line into the `~/.sbgrid.conf` file:

```
PYMOL_M=1.5.0.2
```

Note that entering an **`export=`** command in the bash shell has no effect. The only way to override is by typing the command in this specific form within the `~/.sbgrid.conf` file.

2.4. Software location: `sbwhich`

Software is called in various ways as set-up by the SBGrid system. Some software are in the "PATH" while others are activated via an alias mode. Therefore some of the Unix commands such as **`which`** do not always provide an answer as shown here:

```
$ which rasmol
```

```
/programs/i386-mac/nmrpipe/20130808/nmrbin.mac/rasmol
```

```
$ which pymol
```

```
$ which chimera
```

on the other hand will give only a blank answer because these would have to be searched with another method in "pure" unix sense, with the **`alias`** command:

```
$ alias pymol
```

```
alias pymol='env SB_PYMOLALIAS=pymol /programs/i386-
mac/pymol/pymol-wrapper'
```

```
$ alias chimera
```

```
alias chimera='open /programs/i386-
mac/chimera/1.11/Chimera.app'
```

To remedy this complexity the SBGrid system provides the **`sbwhich`** command that replaces both which and alias commands into a single search mode.

However, note that the results are not identical to the other commands, while still providing accurate information!

```
$ sbwhich chimera
```

```
open /programs/i386-mac/chimera/1.11/Chimera.app
```

```
$ sbwhich pymol
```

```
env SB_PYMOLALIAS=pymol /programs/i386-
mac/pymol/pymol-wrapper
```

```
sbwhich rasmol
```

```
/Volumes/Groups/Software/i386-
mac/rasmol/2.7.5.2/bin/rasmol
```

2.5. Find: `sbgrid-locate`

This command is similar to the Unix **`find`** command but searches only the installed SBGrid.

For example it is possible to find a specific file or the files that are in fact "Apps" as shown (results truncated:)

```
sbgrid-locate "*.app"
```

```
locate: warning: database `/programs/i386-mac/system/db/locate.db' is
more than 60 days old (actual age is 140.6 days)
/programs/i386-mac/2dx/3.1.2/2dx_image/2dx_image.app
/programs/i386-mac/2dx/3.1.2/2dx_logbrowser/2dx_logbrowser.app
/programs/i386-mac/2dx/3.1.2/2dx_merge/2dx_merge.app
/programs/i386-mac/2dx/3.3.0-10.6/2dx_image/2dx_image.app
[truncated]
/programs/i386-mac/xmipp/3.1/external/python/build/tk/Wish Shell.app
/programs/i386-mac/xrayview/4.1/xrayview.app
```

2.6. SBGrid version: `sbinfo`

This utility is mostly useful to report bugs and will reply with information specific to the computer type you are using and the site location. For example the command issued from a Mac will give the following result:

```
$ sbinfo
```

```
/ Operating system: osx-10.11.5-x86_64
Installation name: wisconsin-site
Last update: 20160607
Hostname: BIOCWK-XXXXM
Shell initialization: sh
Software branch: /programs/i386-mac
```

Appendix (2014)

1. List of applications

1.1. SBGrid software directories for Macintosh

2dx	crystfel	gromacs	namd	pytom	solve
3dna	csrosetta	haddock	nedit	qnifft	somore
a2ps	ctf	hbplus	nessy	qpack	sparky
ace2	curves	hkl	netblast	qt	spdbv
adxv	curvesplus	hkl2map	nmrpipe	quilt	specview
aline	delphi	hole	nmrview	r	spider
ambertools	diffmap	ilastik	nuccyl	r2r	spire
amigos2	dino	imagej	nucplot	rasmol	ssaha2
amps	dock	imagemagick	o	raspnmr	staden
apbs	dowser	imod	openbabel	raster3d	stamp
appion	dssp	imosflm	openmotif	raw	suprim
aqua	dssr	imp	openmpi	rcsbtools	surfnet
aria	dynamo	iplt	*osx86.cshrc*	redcat	surfrace
arp_warp	dyndom	isthms	*osx86.shrc*	reduce	surfv
atsas	dyndom3d	jalview	pales	refmac	system
auto3dem	eden	lafire	particle	relax	talosn
autodock	electra	lib	pdb2pqr	relion	tcltk
autoproc	elves	ligplot	perl	remediator	tcoffee
avogadro	em2em	ligplus	pft3dr	replace	tensor
balbes	eman	mafft	pgplot	resmap	theseus
bbhp	eman2	main	phases	ribbons	tkdiff
bfactor	embfactor	mammoth-mult	phenix	ringer	ultrascan
blast	emboss	matt	phoelix	rmeasure	unio
blastplus	emip	mcce	phylip	rmerge	vina
bobscript	entangle	mead	pipe2xeasy	rnamlview	vmd
breseq	epmr	mes	plotmtv	rnaview	wasp
bsoft	espript	mgltools	plotutils	rosetta	whatcheck
buster	fasta	mmc	povray	ruby	wxpython
cara	fastmodelfree	mmtsb	priism	sam	x3d
caver	fftw	modelfree	primer3	saxsview	xds
ccp4	fiji	modeller	probcons	scc	xds-viewer
ccp4mg	finchtv	module	probe	schrodinger	xdsgui
ccpnmr	fpocket	mole	procheck	scwrl4	xdsi
chimera	frealign	molmol	profit	sharp	xdsme
clustal	gamma	molphy	profphd	shelx	xdsstat
cmview	geneious	molscript	promals	shelx-2013	xia2
cns	gerard	mosflm	protskin	signature	xmipp
como	ghostscript	mpich	psipred	simple	xplor
concoord	gnuplot	mrc	pymmlib	simulaid	xrayview
coot	gorgon	mrtailor	pymol	situs	xv
cpmgfit	grace	muscle	pyrosetta	snb	yup
crop	graphviz	naccess	python	solvate	zdock

The list above is that of `/Volumes/Groups/Software/i386-mac`

For up-to-date list of software go to **https://sbgrid.org/software/** or for a complete alphabetical list: **https://sbgrid.org/software/tag/all/**

1.2. Edited short summary of applications

Edited from the list at **https://sbgrid.org/software/**

Software Title	Description	Linux 32-bit	Linux 64-bit	OS X Intel
2dx	A package for data processing of 2DX crystals	✓	✓	✓
3DNA	A package for analyzing, visualizing and rebuilding 3-dimensional nucleic acid structures	✓	✓	✓
a2ps	An Any-to-PostScript filter. It processes plain text files, but also pretty prints quite a few popular languages.	✓	✓	✓
ACE2	A CTF Estimator (ACE) 2. ACE2 is a completely rewritten version of ACE. ACE2 adds the additional feature of robust astigmatism estimation.	✓	✓	✓
ACEMD	ACEMD is heavily optimized molecular dynamics (MD) engine specially designed to run on NVIDA GPUs.		✓	
adxv	Displays protein crystallography X-ray diffraction data. The data may be displayed as a 2-D image, 3-D wire mesh or as integer pixel values.	✓	✓	✓
Aline	An interactive perl/tk application that can read common sequence alignment formats that the user can then alter, embellish, markup, etc.	✓	✓	✓
Alscript	Aprogram to format multiple sequence alignments in PostScript for publication and to assist in analysis.	✓	✓	
AmberTools	AmberTools consists of several independently developed packages that work well by themselves, and with Amber itself. The suite can also be used to carry out complete (non-periodic) molecular dynamics simulations (using NAB), with generalized Born solvent models.	✓	✓	✓
AMIGOS II	Allows the user to perform interactive comparisons between RNA structures and to conduct database searches for specific RNA structures or substructures.	✓	✓	✓
AMPS	A suite of programs designed for the alignment of multiple protein sequences and flexible pattern matching.	✓	✓	✓
APBS	A software package designed for the numerical solution of the Poisson-Boltzmann equation (PBE).	✓	✓	✓
Appion	Appion is a "pipeline" for processing and analysis of EM images.		✓	✓
AQUA	A suite of programs that analyze the quality of biomolecular structures determined via NMR spectroscopy.	✓	✓	✓
ARIA	(Ambiguous Restraints for Iterative Assignment) is a software that automates NOE assignment and NMR structure calculation.	✓	✓	✓
ARP/wARP	An interpretation of crystallographic electron density maps and automatic construction and refinement of macromolecular models.	✓	✓	✓

ATSAS	A program suite for small-angle scattering (SAXS) data analysis from biological macromolecules.	✓	✓	✓
AUTO3DEM	An automated image reconstruction system that coordinates the execution of the parallel, numerically-intensive codes P3DR, PCUT, POR, PPFT, PSF and RobEM (a GUI driven program used both for image preprocessing and visualization).	✓	✓	✓
AutoDock	A suite of automated docking tools. It is designed to predict how small molecules, such as substrates or drug candidates, bind to a receptor of a known 3D structure.	✓	✓	✓
AutoDock Vina	An open-source program for drug discovery, molecular docking, and virtual screening, offering multi-core capability, high performance and enhanced accuracy and ease of use.	✓	✓	✓
autoPROC	autoPROC combines third-party processing programs with new tools and an automated workflow script for automated treatment of multi-sweep X-ray diffraction data.		✓	✓
Avogadro	Avogadro is an advanced molecule editor and visualizer designed for cross-platform use in computational chemistry, molecular modeling, bioinformatics, materials science, and related areas. It offers flexible high quality rendering and a powerful plugin architecture.	✓	✓	✓
BALBES	Aims to integrate into one system all the components necessary for finding a solution structure by MR. It consists of a database, scientific programs and a python pipeline. The system is automated and needs no user intervention when running a complicated combination of jobs, such as model searching, molecular replacement and refinement.	✓	✓	✓
BEST	A program for optimal planning of X-ray data collection from protein crystals.	✓	✓	✓
bfactor	bfactor is a program for filtering 3D maps and applying B-factors.	✓	✓	✓
BioPerl	Acollection of Perl modules that facilitate the development of Perl scripts for bioinformatics applications.	✓	✓	✓
BioPython	A set of tools for biological computation written in Python by an international team of developers.	✓	✓	✓
BLAST	(Basic Local Alignment Search Tool) finds regions of similarity between biological sequences.	✓	✓	✓
BLAST+	(Basic Local Alignment Search Tool) finds regions of similarity between biological sequences.	✓	✓	✓
BnP	Buffalo and Pittsburgh) an interface for complete protein phasing suite includes SnB and Phases.	✓	✓	
BOBSCRIPT	An extension to Molscript	✓	✓	✓
breseq	A computational pipeline for finding mutations relative to a reference sequence in short-read DNA.	✓	✓	✓
Bsoft	A software package written for image processing of electron micrographs, interpretation of reconstructions, molecular modeling, and general image processing.	✓	✓	✓
Burnham-Brandeis Helical Package	A suite of applications for the analysis of helical structures.	✓	✓	✓
BUSTER	BUSTER is a software system for crystallographic structure determination by Bayesian statistical methods		✓	
CARA	An application for the analysis of NMR spectra and compute- aided resonance assignment.	✓	✓	✓
CAVER	CAVER is a software tool for analysis and visualisation of tunnels and channels in protein structures. This is the command line version and not the PyMOL plugin version.	✓	✓	✓
CCP4	(Collaborative Computational Project, Number 4) a collection of programs and associated data and software libraries which can be used for macromolecular structure determination by X-ray crystallography.	✓	✓	✓
CCP4mg	Offers a quick and easy way to create beautiful publication quality images and movies and to superpose and analyze structures.	✓	✓	✓
CcpNmr	An analysis program built on top of the CCP Data Model, inspired partly	✓	✓	✓

	by the program ANSIG (Per Kraulis) and partly by the program Sparky (T.D.Goddard and D.G.Kneller, UCSF).			
CcpNmr ChemBuild	CcpNmr ChemBuild is a graphical tool to construct chemical compound definitions for NMR.	✓	✓	✓
Chimera	A highly extensible, interactive molecular graphics program, often a tool of choice for rendering EM volumes.	✓	✓	✓
Clustal	A general purpose multiple sequence alignment program for DNA or proteins.	✓	✓	✓
CMView	An interactive contact map visualization and analysis tool that supports assessing similarities and differences between structure- or contact predictions.	✓	✓	✓
CNS	An X-ray crystallography suite used for refinement, phasing, and molecular replacement	✓	✓	✓
COMO	Is a program for molecular replacement calculations, using the combined molecular replacement method.	✓	✓	✓
CONCOORD	A method to generate protein conformations around a known structure based on geometric restrictions.	✓	✓	✓
Coot	(Crystallographic Object-Oriented Toolkit) supports model building and real space refinement. The application interfaces with refmac, Phenix, and several other applications. Coot was recognized as the best structural biology application in 2008 by SBGrid.	✓	✓	✓
CPMGFit	A program for non-linear least squares fitting of CPMG relaxation dispersion curves.	✓	✓	✓
crop	A program for cutting sections out of 2D and 3D density maps.	✓	✓	✓
CrystFEL	CrystFEL is a suite of programs for processing diffraction data acquired "serially" in a "snapshot" manner, such as when using the technique of Serial Femtosecond Crystallography (SFX) with a free-electron laser source.		✓	✓
CS-ROSETTA	Chemical-Shift-ROSETTA a robust protocol to exploit mining of protein chemical shifts deposited in the BMRB[…]	✓	✓	✓
CTF	CTFFIND3 and CTFTILT are two programs for finding CTFs of electron micrographs.	✓	✓	✓
Curves+	A complete rewrite of the Curves approach for analyzing the structure of nucleic acids. Included are the helper programs Canal, Cdif and Sumr.	✓	✓	✓
CURVES	An algorithm for calculating a helical parameter description for any irregular nucleic acid segment with respect to an optimal, global helical axis.	✓	✓	✓
CYANA	A program for the automated structure calculation of biological macromolecules on the basis of conformational constraints from NMR. <	✓	✓	✓
DelPhi	A program for calculating protein electrostatics.	✓	✓	✓
Desmond	Software package to perform high-speed molecular dynamics simulations of biological systems on conventional commodity clusters.			
diffmap	diffmap is a program to calculate difference maps between two density maps. The maps must have the same overall dimensions and need to be aligned with each other.	✓	✓	✓
DINO	A realtime 3D visualization program for structural biology data.	✓	✓	✓
DOCK	A molecular docking application.	✓	✓	✓
Dowser	A program that surveys a protein molecule's structure to locate internal cavities and assess the hydrophilicity of those cavities in terms of the energy of interaction of a water molecule with the surrounding atoms.	✓	✓	✓
DPS	(Data Processing Suite) a suite of programs for processing of single crystal X-ray diffraction data of proteins, viruses, nucleic acids and other large biological complexes - emphasis on data collected at synchrotron sources.	✓	✓	
DSSP	A program that standardizes secondary structure assignment calculated from a coordinate file.	✓	✓	✓
DSSR	A software program for Defining the Secondary Structures of RNA from three-dimensional coordinates.		✓	✓

d*TREK	A software suite and toolkit that processes single crystal X-ray diffraction images from two-dimensional position sensitive detectors	✓	✓	✓
Dynamo	A software environment for subtomogram averaging of cryo-EM data.		✓	✓
DynDom	A program to determine domains, hinge axes and hinge bending residues in proteins where two conformations are available.	✓	✓	✓
DynDom3D	A new program to analyze domain movements in large, multi-chain, biomolecular complexes.	✓	✓	✓
Eden	A crystallographic real-space electron-density refinement and optimization program that produces electron density maps with minimal model bias in a robust manner.	✓	✓	✓
Electra	(ELECtron Tomography Resolution Assessment) a suite of programs written to estimate the resolution of electron density volumes obtained by electron tomography.	✓	✓	✓
Elves	Automates most of the repetitive and mindless procedures used in solving macromolecular crystal structures, and is capable of autonomously carrying out all the steps needed to convert raw X-ray diffraction image data to a phased electron density map.	✓	✓	✓
em2em	A program to convert images from/to formats used in the "electron microscopical community" (3DEM)	✓	✓	✓
EMAN	A suite of scientific image processing tools for the transmission electron microscopy community. EMAN includes Foldhunter and Helixhunter.	✓	✓	✓
EMAN2	A scientific image-processing suite with a particular focus on single particle reconstruction from cryoEM images.	✓	✓	✓
EM-BFACTOR	Allows sharpening of high resolution information in 3D maps obtained by electron cryomicroscopy.	✓	✓	✓
EMBOSS	Integrates a range of currently available packages and tools for sequence analysis into a seamless whole.	✓	✓	✓
EM Imaging Processing GUI (EMIP)	(EM Imaging Processing GUI) is a Graphical User Interface written in wxPython that collects information from the user and runs existing programs from a variety of different software packages.	✓	✓	✓
ENTANGLE	A JAVA program that reads PDB files containing a nucleic-acid protein complex and gives a listing of interactions that occur at the interface between the nucleic-acid/protein complex.	✓	✓	✓
EPMR	A program that finds crystallographic molecular replacement solutions using an evolutionary search algorithm. The program directly optimizes three rotational and three positional parameters for the search model with respect to the correlation coefficient between Fo and Fc.	✓	✓	✓
ESCET	A script driven program that analyzes and compares three-dimensional protein structures. The current version (0.7) is mostly designed to find the rigid part of protein molecules by comparing different structures.	✓	✓	
ESPript	(Easy Sequencing in Postscript) is a utility to generate a pretty PostScript output from aligned sequences and coordinate files.	✓	✓	✓
FASTA	A DNA and protein sequence alignment software package that searches for matching sequence patterns or words, called k-tuples. Its legacy is the FASTA format which is now ubiquitous in bioinformatics.	✓	✓	✓
FAST ModelFree	FASTModelFree is a Perl program to assist in the analysis of laboratory frame spin relaxation data. It interfaces with ModelFree 4.01	✓	✓	✓
Fiji	Fiji is an image processing package. It can be described as a distribution of ImageJ (and soon ImageJ2) together with Java, Java 3D and a lot of plugins organized into a coherent menu structure.	✓	✓	✓
FinchTV	FinchTV is the popular way to view DNA sequence traces on Linux, Mac OSX, Windows, and Solaris. FinchTV started as the only chromatogram viewer that can display an entire trace in a scalable multi-pane view. And it leads the way with raw data views, BLAST searching and the ability to reverse complement sequences and traces.	✓	✓	✓
fpocket	fpocket is a very fast open source protein pocket (cavity) detection algorithm based on Voronoi tessellation. It was developed in the C programming language and is currently available as command line driven program.	✓	✓	✓

FREALIGN	(Fourier REconstruction and ALIGNment) a program for high-resolution refinement of 3D reconstructions from cryo-EM images of single particles. A GPU-enabled version is also available.	✓	✓	✓
Gamma	This software is a package of C++ libraries that allow simulation of NMR experiments. It is used for designing and analysing NMR pulse sequences.	✓	✓	✓
GeFREALIGN	FREALIGN is a program for high-resolution refinement of 3D reconstruction from cryoEM of single particles. GeFREALIGN is a version modified to run on GPU processors so that the refinement process of single particle 3D reconstruction can be speedup.		✓	
Geneious	Beautiful sequence alignment, assembly and analysis software. Plans for a permanent 10 seat license provided that number meets current needs.		✓	✓
Ghostscript	An interpreter for the PostScript (TM) language. It can display and convert postscript files. Software can be involved with gs command.	✓	✓	✓
Gnuplot	A portable command-line driven graphing utility originally created to allow scientists and students to visualize mathematical functions and data interactively.	✓	✓	✓
Gorgon	An interactive molecular modeling system specifically geared towards cryo-EM and other low resolution structures of macromolecular complexes.	✓	✓	✓
Grace	A general plotting, curve fitting and data trasformation program.	✓	✓	✓
Graphviz	An open-source graph visualization software program.	✓	✓	✓
Grigorieff Apps	EM utilities from the lab of Niko Grigorieff that include ctffind, ctftilt, bfactor, crop, diffmap and rmeasure.	✓	✓	✓
GROMACS	A versatile package that performs molecular dynamics of proteins, lipids and nucleic acids.	✓	✓	✓
HADDOCK	(High Ambiguity Driven biomolecular DOCKing) relies on an approach that makes use of biochemical and/or biophysical interaction data, such as chemical shift perturbation data resulting from NMR titration experiments, mutagenesis data or bioinformatic predictions.	✓	✓	✓
HBPLUS	A program suite (hbplus, access and clean) to compute hydrogen positions, hydrogen bonds, and neighboring interactions. The application was developed at University College London.	✓	✓	✓
HKL2000	A data processing suite for X-ray crystallography that provides a sleek interface for devising a data collection strategy and processing data. HKL is based on the extended versions of Denzo, Xdisplayf and Scalepack.	✓	✓	✓
HKL2MAP	A graphical user-interface for macromolecular phasing.	✓	✓	✓
HOLE	A program that allows the analysis and visualisation of the pore dimensions of the holes through molecular structures of ion channels.	✓	✓	✓
HYDRONMR	HYDRONMR is a computer program intended for the calculation of NMR relaxation of small, quasirigid macromolecules whose structure, with atomic resolution, is taken from a PDB file of atomic coordintes.	✓	✓	
HYDROPRO	HYDROPRO computes the hydrodynamic properties of rigid macromolecules (proteins, small nucleic acids, macromolecular complexes, etc.) from their structure […] The HYDROPRO calculation comprises the basic hydrodynamic properties: translational diffusion coefficient, sedimentation coefficient, intrinsic viscosity, and relaxation times, along with the radius of gyration.	✓	✓	
ilastik	A simple, user-friendly tool for image classification and segmentation in up to three spatial and one spectral dimension.		✓	✓
ImageJ	It can display, edit, analyze, process, save and print 8-bit, 16-bit and 32-bit images. It can read many image formats including TIFF, GIF, JPEG, BMP, DICOM, FITS and "raw". It supports "stacks", a series of images that share a single window. This installation includes the LOCI BioFormats plugin for reading and editing EM image stacks.	✓	✓	✓
ImageMagick	A software suite to create, edit, compose, or convert bitmap images.	✓	✓	✓
IMOD	A set of image processing, modeling and display programs used for tomographic reconstruction and for 3D reconstruction of EM serial- and optical sections.	✓	✓	✓

iMosflm	A data processing application for macromolecular crystallography. iMosflm (Graphical User Interface) and Mosflm (data processing application) are distributed with this package.	✓	✓	✓
Integrative Modeling Platform (IMP)	is designed to allow mixing and matching of existing modeling components as well as the easy addition of new functionality.	✓	✓	✓
istHMS	An algorithm to reconstruct non-uniformly acquired NMR data.	✓	✓	✓
Jalview	A multiple sequence alignment editor written in Java.	✓	✓	✓
LAFIRE	(Local-correlation-coefficient-based Automatic FItting for REfinement) is an automatic refinement system for protein crystallography.	✓	✓	✓
LigPlot+	A graphical front-end to the LIGPLOT (protein-ligand interactions) and DIMPLOT (protein-protein, domain-domain interactions) programs. The plots generated by these programs can be interactively edited on screen, superposed and printed.	✓	✓	✓
LIGPLOT	A program for automatically plotting protein-ligand interactions.	✓	✓	✓
MadBend	A program for calculating the curvature of nucleic acids to describe the direction and magnitude of a bend angle and can be used to analyze DNA and DNA/protein complex geometries.	✓	✓	
MAFFT	A multiple sequence alignment program. It offers a range of multiple alignment methods, L-INS-i (accurate; for alignment of < 200 sequences), FFT-NS-2 (fast; for alignment of < 10,000 sequences), etc.	✓	✓	✓
MAIN	A model building application for X-ray crystallography.	✓	✓	✓
MAMMOTH-Mult	A package that does multiple alignment of protein structures, providing a common 3D superimposition, a corresponding structure-based sequence alignment and a dendrogram for the set of structures aligned.	✓	✓	✓
Matt	A multiple protein structure alignment program. It uses local geometry to align segments of two sets of proteins, allowing limited bends in the backbones between the segments.	✓	✓	✓
Maxit	to assist in the processing and curation of macromolecular structure data. Features include reading and writing PDB and mmCIF format files, and translating between file formats.	✓	✓	✓
MCCE	(Multi-Conformation Continuum Electrostatics) is a biophysics simulation program combining continuum electrostatics and molecular mechanics.	✓	✓	✓
Mead	A program that is used for including solvation effects in biological systems, such as proteins, using an atomic model of the protein. This is done by solving the Poisson-Boltzmann equation in a dielectric medium, including distributed point charges on a grid.	✓	✓	✓
MES	(Minimal Ensemble Search) a genetic algorithm used to identify the minimal ensemble required to best ï¬t experimental data. The simulations provide an ensemble of molecular models from which a SAXS curve is calculated and compared to the experimental curve.	✓	✓	✓
MGLTools	A software package comprised of AutoDockTools (adt), Python Molecule Viewer (pmv) and a python programming environment called Vision.	✓	✓	✓
MIExpert	An expert system for running molecular replacement and refinement applications, and analyzing the data obtained from high-throughput co-crystallography and fragment screening projects. MIExpert is a module of MIFit.	✓		
MIFit	An interactive graphics application for molecular modeling, fitting, and refinement of protein structures from X-ray crystallography. focus on the efficient solution and analysis of protein:ligand complexes.	✓	✓	
MMC	MMC is a Metropolis Monte Carlo program for the simulation of molecular assemblies in the canonical, grand-canonical and isothermal-isobaric ensembles employing several convergence acceleration techniques		✓	✓
MMTSB Toolset	Multiscale Modeling Tools for Structural Biology	✓	✓	✓
ModelFree	A program to fit the extended model free spectral density function to NMR spin relaxation data.	✓	✓	✓
MODELLER	Is used for homology or comparative modeling of protein three-	✓	✓	✓

	dimensional structures. The user provides an alignment of a sequence to be modeled with known related structures and MODELLER automatically calculates a model containing all non-hydrogen atoms.			
MODULE	A novel program developed to allow the determination of alignment tensor parameters for individual or multiple domains in macromolecules from residual dipolar couplings and to facilitate their manipulation and construct low-resolution models of macromolecular structure.	✓	✓	✓
MOLE	A universal toolkit for rapid and fully automated location and characterization of channels and pores in molecular structures.	✓	✓	✓
MOLMOL	A molecular graphics program for displaying, analyzing, and manipulating the three-dimensional structure of biological macromolecules.	✓	✓	✓
MOLPHY	(MOLecular PHYlogenetics) is a computer program package for molecular phylogenetics.	✓	✓	✓
MolScript	MolScript is one of the most popular programs for the generation of publication-quality figures.	✓	✓	✓
MOSFLM	Apackage for processing film and image plate data.	✓	✓	✓
MRC Cambridge Image Processing System	Determines the structure of macromolecular assemblies. The approach has been to study specimens with some form of symmetry, such as crystals or helical and icosahedral particles, using programs suitable for many kinds of 2-D and 3-D analysis.	✓	✓	✓
mrtailor	PDB preparation tool for use with ProSmart or for Molecular Replacement	✓	✓	✓
MUSCLE	(multiple sequence comparison by log-expectation) is a public domain multiple alignment software for protein and nucleotide sequences.	✓	✓	✓
NACCESS	A stand-alone program that calculates the accessible area of a molecule from a PDB format file.	✓	✓	✓
NAMD	A parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems.	✓	✓	✓
NEdit	A multi-purpose text editor for the X Window System, which combines a standard, easy to use, graphical user interface with thorough functionality and stability.	✓	✓	✓
Nessy	Open source software to analyse NMR relaxation dispersion data of either CPMG or R1p (R1rho) dispersion experiments.	✓	✓	✓
NETBLAST	A simple command-line program that allows you to submit a single file of FASTA sequences over an internet connection to the NCBI BLAST databases. Searches are submitted through the client to the NCBI servers and do not need to download the databases locally (also called netblast and blastcl3).	✓	✓	✓
NMRPipe	A set of comprehensive facilities for Fourier processing of spectra in one to four dimensions, as well as a variety of facilities for spectral display and analysis.	✓	✓	✓
NMRVIEW	Used to visualize and Analyze Nuclear Magnetic Resonance Data.	✓	✓	✓
NORMA	A software suite for the modelling of large conformational changes of 3-D protein structures under the constraint of a low resolution electron density map.	✓	✓	
NUCCYL	A Perl program that allows PyMOL to display atomic models of nucleic acids in a highly simplified representation.	✓	✓	✓
NUCPLOT	A program to generate schematic diagrams of protein-DNA interactions	✓	✓	✓
O	A model building application for X-ray crystallography.	✓	✓	✓
OpenBabel	Search, convert, analyze, or store data from molecular modeling, chemistry, solid-state materials, biochemistry, or related areas.	✓	✓	✓
PARTICLE	A software package for single-particle EM image processing with comprehensive data analysis functions for particle selection, particle classification, 3D reconstruction and model evaluation.		✓	✓
PDB2PQR	A Python software package providing a platform-independent utility for converting protein files in PDB format to PQR format.	✓	✓	✓
pdb-care	Able to identify and assign carbohydrate structures using only atom types and their 3D atom coordinates given in PDB-files.		✓	

PDB_REDO	PDB_REDO refines any structural model you are working on, by optimising REFMAC refinement and by partial model rebuilding.		✓	
PDB Validation Suite	A set of tools used by the PDB for processing and checking structure data.	✓	✓	✓
Perl	Script Language.	✓	✓	✓
PFT3dr	Performs orientation searches and positional refinement of icosahedral viruses.	✓	✓	✓
PGPLOT	AFortran- or C-callable, device-independent graphics package for making simple scientific graphs.	✓	✓	✓
PHASES	Computes phase angles for diffraction data from macromolecular crystals.	✓	✓	✓
PHENIX	(Python-based Hierarchical Environment for INtegrated Xtallography) provides tools for automated structure solution by X-ray crystallography.	✓	✓	✓
PHOELIX	A software package for image processing of helical macromolecular complexes.	✓	✓	✓
PHYLIP	A free package of software programs for inferring phylogenies.	✓	✓	✓
pipe2xeasy	Performs conversions of spectra from NMRPipe to XEASY format.	✓	✓	✓
PLOTMTV	PLOTMTV is a multipurpose X11 plotting program and specializes in contour plots, but it can also handle 2D and 3D plots.	✓	✓	✓
plotutils	A GNU package containing software for programmers and technical users. Its centerpiece is libplot, a powerful C/C++ function library for exporting 2-D vector graphics in many file formats, both vector and raster	✓	✓	✓
POVRAY	(Persistence of Vision Raytracer) is a high-quality, totally free tool for creating stunning three-dimensional graphics.	✓	✓	✓
Prediction of ALignmEnt from Structure (PALES)	A software for the analysis of residual dipolar couplings. Its main component is the PALES (Prediction of ALignmEnt from Structure) simulation that predicts the magnitude and orientation of a sterically induced alignment tensor from a solute's (protein/nucleic acid/oligosaccharide) three-dimensional shape.	✓	✓	✓
Priism/IVE	Graphical interface to a collection of applications for the analysis and visualization of multidimensional data, with a focus on data from 3D optical microscopy and electron tomography. IVE (Image Visualization environment) is the core set of software libraries that are the foundation for the tools in Priism.	✓	✓	✓
Primer3	A widely used program that designs PCR primers (PCR = "Polymerase Chain Reaction"). Primer3 can also design hybridization probes and sequencing primers.	✓	✓	✓
PROBCONS	An efficient protein multiple sequence alignment program, which has demonstrated a statistically significant improvement in accuracy compared to several leading alignment tools.	✓	✓	✓
Probe	An application to evaluate atomic packing, either within or between molecules. It generates *contact dots* where atoms are in close contact	✓	✓	✓
PROCHECK	Checks the stereo-chemical quality of a protein structure, producing a number of PostScript plots analyzing its overall and residue-by-residue geometry.	✓	✓	✓
ProFit	The ultimate protein least squares fitting program.	✓	✓	✓
PROFphd	A new package added as part of the pipeline to create fragments for Rosetta.	✓	✓	✓
PROMALS	(PROfile Multiple Alignment with predicted Local Structure) is a progressive method for aligning multiple protein sequences, with enhanced profile information from database searches and secondary structure prediction.	✓	✓	✓
PROSPECT	A threading-based protein structure prediction system.	✓	✓	
Protomo	Includes programs and shell scripts for electron tomography of thin specimens.	✓	✓	
ProtSkin	Converts a protein sequence alignment in BLAST, CLUSTAL or MSF format to a property file used to map the sequence conservation onto the structure of a protein using the GRASP program or the MOLMOL program	✓	✓	✓

	or the PyMOL program			
PSIPRED	Uses a simple and accurate secondary structure prediction method incorporating two feed-forward neural networks which perform an analysis on output obtained from BLAST.	✓	✓	✓
PyMOL	Widely used molecular visualization package developed by Warren DeLano, and now maintained by Schödinger, LLC.	✓	✓	✓
PyRosetta	An interactive Python-based interface to the powerful Rosetta molecular modeling suite. It enables users to design their own custom molecular modeling algorithms using Rosetta sampling methods and energy functions.	✓	✓	✓
Python	A programming language that lets you work more quickly and integrate your systems more effectively.	✓	✓	✓
Python Macromolecular Library	Is a software toolkit and library of routines for the analysis and manipulation of macromolecular structural models, implemented in the Python programming language.		✓	✓
PyTOM	PyTom unifies standard tomogram processing steps in a single python-based toolbox.	✓	✓	✓
Qnifft	Software for macromolecular electrostatics.	✓	✓	✓
QPack	A "quick" evaluation of steric packing in protein structures.	✓	✓	✓
QUILT	Detects contiguous stretches of hydrophobic surface area on the surfaces of macromolecules.	✓	✓	✓
R	A free software environment for statistical computing and graphics.	✓	✓	✓
R2R	R2R is a program to assist in aesthetic drawings of RNA secondary structures. It is primarily aimed at drawing consensus diagrams, but can also draw single RNA molecules.	✓	✓	✓
Rasmol	A molecular graphics program intended for the visualisation of proteins, nucleic acids and small molecules.	✓	✓	✓
RASPnmr	(Protein NMR backbone resonance assignment) uses structure-based chemical shift predictions to solve the backbone resonance assignment problem in protein NMR spectroscopy.		✓	✓
Raster3D	A set of tools for generating high quality raster images of proteins or other molecules.	✓	✓	✓
RAW	BioXTAS RAW is a program for analysis of Small Angle X-ray Scattering data.	✓	✓	✓
RCrane	Allows for semi-automated building of RNA structure within Coot.	✓	✓	✓
REDCAT	A residual dipolar coupling analysis tool.	✓	✓	✓
Reduce	A program for adding hydrogens to a Protein DataBank (PDB) molecular structure file.	✓	✓	✓
REFMAC	Carries out rigid body, tls, restrained or unrestrained refinement against Xray data, or idealisation of a macromolecular structure. It minimises the coordinate parameters to satisfy either a Maximum Likelihood or Least Squares residual.	✓	✓	✓
relax	Molecular dynamics by NMR data analysis. relax is a program designed for the study of the dynamics of proteins or other macromolecules though the analysis of NMR relaxation experiments.	✓	✓	✓
RELION	(REgularised LIkelihood OptimisatioN) is a stand-alone computer program for Maximum A Posteriori (MAP) refinement of (multiple) 3D reconstructions or 2D class averages in cryo-electron microscopy.	✓	✓	✓
Remediator	Converts PDB files between PDBv2.3 and PDBv3.2 formats	✓	✓	✓
REPLACE (GLRF and TF)	A suite of programs for molecular replacement calculations. It currently consists of two major programs, GLRF for rotation function calculations and TF for translation function calculations. In addition, a small program (ANGCAL) is a convenient tool for conversions between angles and matrices.	✓	✓	✓
ResMap	Software package for computing the local resolution of 3D density maps studied in structural biology, primarily electron cryo-microscopy (cryo-		✓	✓

	EM).			
Ribbons	A popular molecular graphics software display package.	✓	✓	✓
Ringer	A program to detect molecular motions by automatic electron density sampling.	✓	✓	✓
rmeasure	A program for measuring the resolution of single-particle reconstructions.	✓	✓	✓
RMERGE	RMERGE can calculate Rpim for merging, which HKL (scalepack) does not. There's no official manual right now but you can see Cell 147, 199-208 for more information.	✓	✓	✓
RnamlView	RnamlView is a visualization tool that displays/edits 2-dimensional diagrams of RNA/DNA secondary structures with tertiary interactions created by RNAView.	✓	✓	✓
RNAView	Quickly display the secondary structure of RNA/DNA with tertiary interactions.	✓	✓	✓
Rosetta	A software suite for predicting and designing protein structures, protein folding mechanisms, and protein-protein interactions.	✓	✓	✓
RSRef2000	Supports real-space simulated annealing refinement with X-ray data.	✓	✓	
Ruby	A dynamic, open source programming language with a focus on simplicity and productivity. It has an elegant syntax that is natural to read and easy to write.	✓	✓	✓
SAM	A collection of tools for creating, refining, and using linear hidden Markov models for biological sequence analysis	✓	✓	✓
saxsview	A plotting facility for SAXS-data, as well as a convenient tool to quickly generate plots for publication.	✓	✓	✓
SCC	A suite of programs for sequence alignment including: aln, swg, prrn, phyln and makmdm.	✓	✓	✓
Schrodinger Suite	A suite of tools for small molecule drug discovery but due to it's size, it is not included in our default installation.	✓	✓	✓
SCWRL3	Program for prediction of protein side-chain conformations.	✓	✓	
SCWRL4	Program for prediction of protein side-chain conformations.	✓	✓	✓
SHARP/autoSHARP	An automated structure solution pipeline built around the heavy-atom refinement and phasing program SHARP, the density modification program SOLOMON, and the ARP/wARP package for automated model building and refinement (using REFMAC).	✓	✓	✓
SHELX-2013	A set of programs for macromolecular phasing.	✓	✓	✓
SHELX-97	A set of programs for macromolecular phasing.	✓	✓	✓
SIGNATURE	An automated particle selection system for electron microscopy.	✓	✓	✓
SIMPLE	Single-particle IMage Processing Linux Engine (SIMPLE) does ab initio 3D reconstruction (programs cluster & origami), heterogeneity analysis (programs cluster, origami & cycler), and high-resolution refinement (programs align, reconstruct, automask & cycler).		✓	✓
Simulaid	A collection of utilities designed to help setting up and analyze molecular simulations.		✓	✓
SITUS	A program package for modeling of atomic resolution structures into low-resolution density maps. The software supports both rigid-body and flexible docking using a variety of fitting strategies.	✓	✓	✓
SnB	Determination of the anomalously scattering substructures of selenomethionyl-substituted proteins containing as many as 160 Se sites.	✓	✓	✓
Solvate	A program to construct an atomic solvent environment model for a given atomic macromolecule model (solute) for use in molecular dynamics simulations.	✓	✓	✓
SOLVE/RESOLVE	A program that can automatically search for heavy atom sites, calculate initial phases and perform density modification.	✓	✓	✓
SOMoRe	6D global search and multi-start optimization molecular replacement package.	✓	✓	✓
Sparky	A graphical NMR assignment and integration program for proteins, nucleic acids, and other polymers.	✓	✓	✓

SPARX	(Single Particle Analysis for Resolution eXtension) is an image processing environment with a particular emphasis on transmission electron microscopy (TEM) structure determination.	✓	✓	✓
SpecView	Designed to provide a fast way to visualise NMR spectrum and peak data. It supports 2D and 3D graphical display modes for multidimensional and simple 1D spectra.	✓	✓	✓
SPIDER	(System for Processing Image Data from Electron microscopy and Related fields) is a large image processing suite for electron microscopy.	✓	✓	✓
Spire	A graphical user interface for executing SPIDER batch files and other programs.	✓	✓	✓
SSAHA2	(Sequence Search and Alignment by Hashing Algorithm) is a pairwise sequence alignment program designed for the efficient mapping of sequencing reads onto genomic reference sequences.	✓	✓	✓
Staden	A set of DNA sequence assembly, editing and analyzing tools.	✓	✓	✓
STAMP	(STructural Alignment of Multiple Proteins) a suite of programs for the comparison and alignment of protein three-dimensional structures.	✓	✓	✓
Suprim	A software package intended primarily for the processing of transmission electron micrographs.	✓	✓	✓
Surface Racer	Calculates exact accessible surface area, molecular surface area and average curvature of molecular surface for macromolecules. The program also analyzes cavities in the protein interior inaccessible to solvent from outside.	✓	✓	✓
SURFNET	A program that generates surfaces, density contours and gap regions from coordinate data supplied in a PDB file.	✓	✓	✓
surfv	Calculates solvent accessible area that is defined by a probe as it rolls on the surface of the molecule. Thus use of a zero radius probe will give the Van der Walls surface area.	✓	✓	✓
Swiss-PdbViewer	An application that provides a user friendly interface allowing you to analyze several proteins at the same time.	✓	✓	✓
TALOS-N	TALOS-N: Prediction of Protein Backbone and Sidechain Torsion Angles from NMR Chemical Shifts		✓	✓
T-Coffee	A multiple sequence alignment package. You can use T-Coffee to align sequences or to combine the output of your favorite alignment methods (Clustal, Mafft, Probcons, Muscle...) into one unique alignment (M-Coffee).	✓	✓	✓
TENSOR	Allows the determination of rotational diffusion from three-dimensional structure coordinates and experimental 15N relaxation data, and nowallows a rigorous model-free analysis of local internal mobility affecting backbone amides, from 15N {R1,R2,nOe} relaxation rates in the presence of an isotropic of anisotropic rotational diffusion tensor.	✓	✓	✓
The Image Processing Library & Toolbox (IPLT)	A 2D Crystallography Suite developed by Andreas Schenk.	✓	✓	✓
Theseus	A program that simultaneously superimposes multiple macromolecular structures using the method of maximum likelihood. By downweighting variable regions of the superposition and by correcting for correlations among atoms, the ML superpositioning method produces much more accurate results.	✓	✓	✓
THREADER	Offers protein fold recognition by optimal protein sequence threading.	✓	✓	
Tiltpicker	A graphical user interface for picking particles from image tilt pairs for such applications as random conical tilt (RCT) and orthogonal tilt reconstruction (OTR).	✓	✓	
TkDiff	A graphical front end to the diff program. It provides a side-by-side view of the differences between two files, along with several innovative features.	✓	✓	✓
ULTRASCAN2	A software package offering comprehensive analysis of hydrodynamic data from analytical ultracentrifugation experiments.	✓	✓	✓
ULTRASCAN3	The latest multi-platform version of UltraScan, which is has now replaced the UltraScan II distribution.	✓		✓

UNIO	UNIO enables you to perform automated NMR data analysis for protein 3D structure determination.	✓	✓	✓
Untangle	A program designed to separate overlapping diffraction patterns from a set of crystals with slightly different orientations.	✓	✓	
UROX	UROX is deprecated, a new version named VEDA should be used instead	✓	✓	
USF Gerard Utilities	The Swiss Army knife of crystallography tools. The installation includes the packages from RAVE, SBIN, X-UTIL, VOIDOO, DEJAVU and SPASM.	✓	✓	✓
VEDA	VEDA is a visual environment developed to fit interactively atomic models into 3D reconstructions. Calculations are performed in reciprocal-space and the symmetry of the reconstruction is taken into account. The computations are fast and an entire EM reconstruction can be used.	✓	✓	
VMD	A molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting.	✓	✓	✓
vmd-xplor	The vmd-xplor package is a combination of the X-PLOR structure determination program and VMD (Visual Molecular Dynamics) that allows manual manipulation of the protein structures to satisfy experimental NMR data. It can also be used to visualize the goodness of fit of a particular model to given restraints.	✓	✓	✓
WASP	Searches PDB files for misidentified water molecules that should be modeled as cations.	✓	✓	✓
Wattos	A collection of Java programs for structural biology and NMR spectroscopy that analyze, annotate, parse, archive, and disseminate experimental NMR data deposited worldwide into the PDB and BMRB.	✓	✓	
WHAT_CHECK	The protein verification tool from the WHAT IF program available as a free stand-alone program, complete with all source code.	✓	✓	✓
WHATIF	A general protein analysis program.	✓	✓	
X3D	X3D is a boxing program developed by James Conway.	✓	✓	✓
XDP	Used for processing Electron Diffraction data.	✓	✓	
XDrawChem	A two-dimensional molecule drawing program for Unix operating systems that can read and write MDL Molfiles, and read ChemDraw text and binary files, to allow sharing between XDrawChem and other chemistry applications, and it can create images in popular formats like PNG and EPS.	✓	✓	
XDS	X-ray Detector Software for processing single-crystal monochromatic diffraction data recorded by the rotation method. Written by Wolfgang Kabsch (see Tales about Developers section on SBGrid website).	✓	✓	✓
XDSAPP	A graphical user interface for the easy and convenient processing of diffraction data sets using XDS.	✓	✓	✓
XDSGUI	XDSGUI is a GUI (graphical user interface) for XDS that is supposed to help both novice and experienced users.	✓	✓	✓
XDSi	Allows processing of datasets in a given directory with minimum effort.	✓	✓	✓
xdsme	xdsme is a collection of python scripts made to simplify the processing of crystal diffraction images with the XDS Program.	✓	✓	✓
XDSSTAT	A home-brewed program that prints various statistics (that are not available from XDS itself) in the form of tables and images.	✓	✓	✓
XDS-Viewer	An X-ray diffraction and control image viewing utility for data processed using the XDS program package.	✓	✓	✓
XEASY	A program for interactive, computer-supported NMR spectrum analysis.	✓	✓	
XIA2	An automated data reduction system designed to work from raw diffraction data and a little metadata to immediately start phasing and structure solution.	✓	✓	✓
Xmipp	(X-Window-based Microscopy Image Processing Package) a suite of image processing programs primarily aimed at single-particle 3D electron microscopy.	✓	✓	✓
Xplor-NIH	A system for X-ray crystallography and NMR.	✓	✓	✓

XRayView	Uses interactive computer graphics to introduce basic concepts of X-ray diffraction by crystals, including the reciprocal lattice, the Ewald sphere construction, Laue cones, the wavelength dependence of the reciprocal lattice etc.	✓	✓	✓
xv	xv is an interactive image manipulation program for the X Window System. It can operate on images in the GIF, JPEG, TIFF, PBM, PGM, PPM, XPM, X11 bitmap, Sun Rasterfile, Targa, RLE, RGB, BMP, PCX, FITS, and PM formats on all known types of X displays.	✓	✓	✓
YUP	(Yammp Under Python) is a molecular modeling program designed as a general purpose tool currently concentrated on molecular simulations (mechanics) and on reduced representation and multiscale modeling.	✓	✓	✓
ZDOCK/RDOCK	Two protein docking algorithms designed to operate in succession. ZDOCK is a rigid-body docking program, and RDOCK is a refinement program.	✓	✓	✓
Zephyr	A tool for analyzing and manipulating images, especially those generated for electron microscopy. Zephyr is scriptable in Python.	✓	✓	
ZINC	A free database of commercially-available compounds for virtual screening. ZINC contains over 21 million purchasable compounds in ready-to-dock, 3D formats.			

1.3. Index

This is a dummy index, left here purely to store the format.

No index entries found.