

CRYSTALLOGRAPHY SOFTWARE AT THE SBC

Where?

On SBC Linux machines, application software is organized in version-specific subdirectories under **/net/prog1**.

How?

For command line suites, you need to type XXX-setup (where XXX represents the desired application), which will give you an xterm from which you can run the XXX program commands.

For GUIs, and a subset of specific programs, type the command scripts located under **/net/prog1/bin**.

Command scripts are in your path for the following programs:

FOR:	TYPE AT THE PROMPT: (CASE SENSITIVE)
GUI interfaces	
ARP/wARP	ccp4i
ccp4i	ccp4i
Coot	coot
hkl2map (shelx)	hkl2map
HKL3000	HKL3000
Mosflm	mosflm, imosflm
O	ono
phenix	phenix
PyMOL	pymol
SnB	SnB
XtalView	xfit, xtalmgr, or ccp4i
xprep	xprep
Command line suites**	
CCI Apps (phenix.xtriage, phenix.hyss, etc.)	cci-setup
CCP4	ccp4-setup
CNS	cns-setup
SHELX-97	shelx-setup
Solve/Resolve	solve-setup
Some USF programs	
dataman	dataman

mapman	mapman
moleman	moleman
moleman2	moleman2
Seq2comp.f	seq2comp

**The setup scripts produce a light gray xterm. Within this window, the suite should be fully functional.

WEB SITE LINKS FOR CRYSTALLOGRAPHERS

APS Storage Ring Status

<http://www.aps.anl.gov/aod/blops/status/smallHistory.html>

BnP

<http://www.hwi.buffalo.edu/BnP/>

Book of Fourier

<http://www.ysbl.york.ac.uk/~cowtan/fourier/fourier.html>

CCI Apps

http://www.phenix-online.org/download/cci_apps

CCP4

<http://www.ccp4.ac.uk/>

CNS

<http://cns.csb.yale.edu/v1.2/>

COOT

<http://www.ysbl.york.ac.uk/~emsley/cool/>

European Bioinformatics Institute

<http://www.ebi.ac.uk/>

ExpASy Proteomics Server

<http://ca.expasy.org/>

HKL

<http://www.hkl-xray.com/>

MolProbity

<http://molprobity.biochem.duke.edu/>

mosflm

<http://www.mrc-lmb.cam.ac.uk/harry/mosflm/>

NCBI

<http://www.ncbi.nlm.nih.gov/>

O

<http://xray.bmc.uu.se/~alwyn/>

PDB

<http://www.rcsb.org/pdb/Welcome.do>

Protein Crystallography Course

<http://www-structmed.cimr.cam.ac.uk/course.html>

PyMOL

<http://pymol.sourceforge.net/>

SHELX

<http://shelx.uni-ac.gwdg.de/SHELX/>

SnB

<http://www.hwi.buffalo.edu/SnB/>

Solve/Resolve

<http://www.solve.lanl.gov/>

TargetDB

<http://targetdb.pdb.org/>

Twining server

<http://nihserver.mbi.ucla.edu/Twining/>

Uppsala Software Factory

<http://xray.bmc.uu.se/usf/>

X-ray Anomalous Scattering

http://www.bmsc.washington.edu/scatter/AS_index.html

XtalView

<http://www.sdsc.edu/CCMS/Packages/XTALVIEW/XVcprt.html>

MEC December 2007