

pdb2pov

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REVISION HISTORY

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Chapter 1

pdb2pov

1.1 pdb2pov.guide

pdb2pov

This document describes pdb2pov, a program written by Eric G. Suchanek, Ph.D. The program has been designed to allow the user to quickly and easily convert Brookhaven data bank format files to 'POV-Ray' v2.0 format scene files on the Amiga personal computer. The program has a wide variety of options which can be used to produce some stunning images. This program is used primarily by my program 'CPK', but may be used as a stand-alone application.

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1.2 pdb2pov.guide/Legal

Legal/Disclaimer

You may distribute this program freely as long as it is not "For Profit", and as long as all files in the distribution remain intact. Fred Fish is expressly given permission to distribute this code in his disk collection.

This program is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. Use at your own risk!

I consider this program to be 'CharityWare'. If you like it, please consider sending a donation to the National SIDS foundation. You can

read more about SIDS in the About.SIDS document included in this distribution.

1.3 pdb2pov.guide/Purpose

Program Description

PDB2POV is a CLI program designed to convert Brookhaven format atomic structure files into POV-Ray Version 2.0 compatible scene files. The program has a large number of options to change the atomic rendering style for CPK, van der Waals, or covalent radii spheres. The user may also specify two ground styles (plain or checkerboard), area light sources, and a nice cloudy sky. Finally, the user may specify for X, Y, and Z axis rotations to orient the molecule.

The molecular format used is called 'Protein Data Bank' (.pdb) format. This is one of the most prevalent formats used in modern chemistry. The entire Protein Data Bank consists of a few hundred protein and DNA molecular structures and can be obtained from the Brookhaven laboratories for a nominal fee (or from me if you know what you want).

This program was designed to be used with my molecular rendering program CPK, but may be used manually as well.

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1.4 pdb2pov.guide/Distribution

Distribution

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In addition to the program, this distribution includes a number of atomic 'include' files to be used with the generated scene files.

You should have received:

- * 'pdb2pov.000' - 68000 optimized version (IEEE math)
- * 'pdb2pov.030' - 68030 optimized version (IEEE math)
- * 'pdb2pov.040' - 68040 optimized version (68882 math)
- * 'Pdb2POV.dvi|guide' - this file

- * 'About.Sids' - documentation about the SIDS foundation
- * 'crambin.pdb' - a small protein molecule
- * 'crambin.pov' - 'POV-Ray' V2.x scene file from crambin.pdb
- * 'atoms2.inc' - main atom include file (shiny plastic)
- * 'atoms_covalent.inc' - covalent atomic radii include file
- * 'atoms_cpk.inc' - CPK radii atomic include file
- * 'atoms_vdw.inc' - van der Waals radii atomic include file
- * 'atoms_glass2.inc' - atom definitions with 'glass' texture
- * 'babel' - a program to convert atomic format files
- * 'babel.doc' - documentation for the 'babel' program
- * '#?.lis' - additional files for the 'babel' program

1.5 pdb2pov.guide/Requirements

Requirements for running 'pdb2pov'

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This program should run on any Amiga. There are no operating system specific calls, so I wouldn't be surprised if it runs under 'v1.3'. I have not tested this, however. The program uses dynamic memory allocation to read the atomic structures, and should gracefully exit if it runs out of memory. I would recommend at least 1MB RAM memory in order to read relatively large structure files.

You will, of course, need a copy of 'POV-Ray' version 2.0 or higher. This is an excellent public domain ray-tracer which may be found on a number of BBS and internet sites.

NOTE: I have customized 'POV-Ray' to be slightly more compatible with the current version of CPK. My version also has direct support for the Picasso II RTG 24 bit graphics board. This version is available on aminet and BIX. The name will be 'povami_picasso_xx.lha', where xx represents an internal version number.

1.6 pdb2pov.guide/Installation

Installation

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1. Drag the 'pdb2pov' drawer to some appropriate location on your

system.

2. Copy all files from the include directory to your normal 'POV-Ray' include area.

1.7 pdb2pov.guide/Usage

Usage

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If you just type the program name with no arguments you should see a USAGE message something like:

```
Program: $Id: pdb2pov.texinfo,v 1.4 1995/01/27 20:11:08 eric Exp $
```

```
USAGE: pdb2pov.040 InputFile OutputFile
      [-o object_only]
      [-t atm file format]
      [-p (no sky or ground)]
      [-s (writes cloudy sky)]
      [-g (writes plain ground)]
      [-h (writes checkered ground)]
      [-a (create area light)]
      [-v (do van der Waals radii)]
      [-c (do covalent radii)]
      [-b (do ball_and_stick)]
      [-d (bond cutoff threshold)]
      [-q (ball and stick + glass atoms)]
      [-x X-Axis rotation]
      [-y Y-Axis rotation]
      [-z Z-Axis rotation]
```

```
      Author: Eric G. Suchanek, Ph.D.
      All rights reserved
```

The options are as follows:

- * -o - Only write the object definition with no ground or sky
 - * -t - Read the input format in Tripos .atm format rather than the default Brookhaven pdb format
 - * -p - Don't generate any sky or ground at all
 - * -s - Generate statements for a nice cloudy sky background
 - * -g - Generate statements for a bumpy dark purple 'plain' ground
 - * -h - Generate statements for the classic checked ground
 - * -a - Generate statements for an 'area light' light source. These produce soft shadows but can take a very long time to render.
 - * -v - Render the scene with van der Waals atomic radii
-

- * -c - Render the scene with covalent atomic radii
- * -b - Render the scene in ball and stick mode
- * -d - Specify the distance (Angstroms) above which bonds will not be generated for ball and stick mode.
- * -q - Generate a hybrid molecule with ball and stick atoms overlaid with glass spheres. This looks really good, but takes an extremely long time to render.
- * -x - Specify an X-Axis rotation angle (degrees).
- * -y - Specify a Y-Axis rotation angle (degrees).
- * -z - Specify a Z-Axis rotation angle (degrees).

The `*InputFile*` and `*OutputFile*` parameters are assumed to have extensions of `'.pdb'` and `'.pov'`, respectively, so don't specify any extensions on the command line.

Here's an example:

```
pdb2pov.040 crambin crambin -s -h -x 90 -b -d 1.8
```

This would take `'crambin.pdb'` to `'crambin.pov'`, generate sky and checkered ground, rotate the molecule 90 degrees in the X axis, and generate ball and stick mode with a distance cutoff of 1.8 Angstroms.

The program tries to be intelligent about positioning the molecule so that the whole structure is within the field of view, but you're naturally free to adjust the position by hand for more aesthetic results if you wish.

You may also use the atomic radii flags (`'-v -c'`) to get different effects. By using the `'-v'` flag you'll get van der Waals radii spheres, and `'-c'` will use covalent radii. The default is to use approximate CPK radii.

Finally, a note about `*ball and stick mode*`. The program uses a bond distance cutoff of 2.0 angstroms for computing bonds. That is, any distance greater than this will not be considered a bond. If you find yourself getting lots of spurious bonds try decreasing this value. The default is generally reasonable for 'typical' atomic structures, though.

If the program can't recognize a specific atom type it will use the parameters for `'carbon'`. You may therefore need to edit the scene file or add to `'atoms2.inc'`, `'atoms_glass2.inc'` and the radii files. If you update these files please send me a copy.

1.8 pdb2pov.guide/Miscellaneous

Miscellaneous

The Brookhaven data bank

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The Brookhaven data bank is one of the principal repositories for protein and nucleic acid crystallographic structures. The lab maintains an anonymous FTP site at: 'pdb.pdb.bnl.gov', (130.199.144.1).

This site has the current structure database as well as a number of useful programs. Brookhaven also distributes a quarterly CD-ROM with the latest database. Send E-Mail to 'pdb@chm.bnl.gov' for ordering information.

Babel

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Babel

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Many people have requested the capability of reading and converting more than just 'PDB' files from 'pdb2pov'. However, adding a good assortment of molecular file filters is not trivial. I am now including the program 'Babel' with this distribution. 'Babel' was written by Pat Walters and Matt Stahl; the program can read and write a wide variety of atomic structure file formats. For more information on 'Babel' see the file 'Babel.doc'.

1.10 pdb2pov.guide/Macintosh Version

Macintosh version

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Richard Rothwell has kindly ported 'pdb2pov' to the Macintosh and has made the binaries available on the official POV-Ray distribution site, *ftp.povray.org*. You may contact him at *chergr@lure.latrobe.edu.au* for more information on this port.

1.11 pdb2pov.guide/Program History

Program History

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- * V1.21 - Unification of changes for the Macintosh port by Richard Rothwell, email: chergr@lure.latrobe.edu.au
- * V1.20 - Internal release only
- * V1.18 - Some minor radii changes, now includes correct 'babel' include files. Also changed so that the 68000 and 68030 versions use the IEEE library. Only the '040 version uses the math coprocessor.
- * V1.17 - Minor bug fix in 68000 version. Wasn't calculating the bond table correctly. March, 1994.
- * V1.16 - Added ball and stick mode. January, 1994
- * V1.15 - First public release, December 1993

1.12 pdb2pov.guide/Concept Index

Concept Index

This section contains a list of general topics (or **concepts** in Texinfo parlance) derived from this document.

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