

BRAGI



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Introduction

BRAGI is originated during Prof. Schomburg time at the GBF and is now developed in cooperation between the GBF in Braunschweig and the University of Cologne.

If you use BRAGI in your publications please use the following reference:

D. Schomburg and J. Reichelt, BRAGI: A comprehensive protein modeling program system. *J. Mol. Graphics*, Vol. 6, pages 161-165, 1988

What is BRAGI?

BRAGI is an interactive protein modeling program. It was developed for the special purpose to model unknown proteins from the structure of a known one. BRAGI enables you to view and explore the three-dimensional (3D) structure of any macromolecule. You can explore proteins, DNA, RNA, carbohydrates, and complexes, such as between transcriptional regulatory proteins and DNA, or enzymes and drugs. BRAGI includes also a set of programs and utility functions.

The software:

BRAGI is entirely written in C/C++ and the graphics is using OpenGL. The windowing and the scripting are implemented using Qt. The Qt scripts defining the graphics layout are plain XML files and can thus very easily be modified. You can import, display and analyze several different input coordinate file formats. The program has a graphical user interface (GUI) based on Qt.

Requirements to run BRAGI

The BRAGI program is currently supported on the following platforms:

- Windows 98/2000/XP
 - Windows 98 must have all patches installed as were available late 2003
 - Windows 2000 must have service pack 4 installed
 - Windows XP must have service pack 1 installed
- Linux:
 - at now we have tested
 - SuSE 8.x, 9.0
 - Fedora Core 1
 - Mandrake
- SGI IRIX 6.5

The main platforms are Windows and Linux.

A rough guess is that you need at least 32 MB of memory. To install on disk you need about 600 MB. No special graphics hardware is needed for the Windows and Unix/Linux versions. The usual graphics cards on the Windows platform gives a very convenient rendering speed. To be able to render acceptable graphics quality it is recommended that you run your display in either 16 bit graphics mode (64 K colors) or in the true color mode (16 M colors). To get really nice stereo graphics support you must have a graphics card that support hardware stereo, e.g on PC systems NVIDIA Quadro boards. Don't forget to by a card with a plug for the stereo glasses!

Supported file formats:

Currently BRAGI supports the molecular coordinate input format of PDB (Protein Data Bank format).

Limited import of mol2 files is build in. BRAGI uses only two block of this file: "@<TRIPOS>ATOM" and "@<TRIPOS>BOND". All atoms of a residue must be written together. So it is not allowed to put the hydrogens of a protein at the end of the "@<TRIPOS>ATOM" block. This will result in doubling all residues. There may be more than one molecule in one file.

To read in files in another format, we suggest using "Open Babel" from <http://openbabel.sourceforge.net/>

BRAGI as a helper application for your Web browser:

It is possible to use BRAGI as a helper application to your favorite Unix/Linux/Windows Web browser. Please look into your favorite Web browser setup on how to start **BRAGI**. At now BRAGI is not implemented to work as a plugin.

Introduction to BRAGI

BRAGI may run directly from CD, or you may copy the whole CD to any directory on your hard disk. Some functions need write access to this directory tree, e.g. saving of topologies.

Before we look at the GUI in more detail it is worth describing some of the things you don't see but yet they are still there:

- When BRAGI runs it reads a lot of information about residues etc., which will be needed for the display or other purposes.
- The user can modify a lot of the default parameters or variables at startup through two startup files:
 1. At startup bragi reads first the system startup file (**bragi.set**) located in the bragi/ directory. This file contains information related rather to all users.
 2. The second file is **.bragi.set** from your login directory, which can contain information specific for one user.
 3. The third file is .bragi.set in actual working directory where you started BRAGI from.

To start BRAGI on the WIN32 platform
run the **bragi.exe** file.

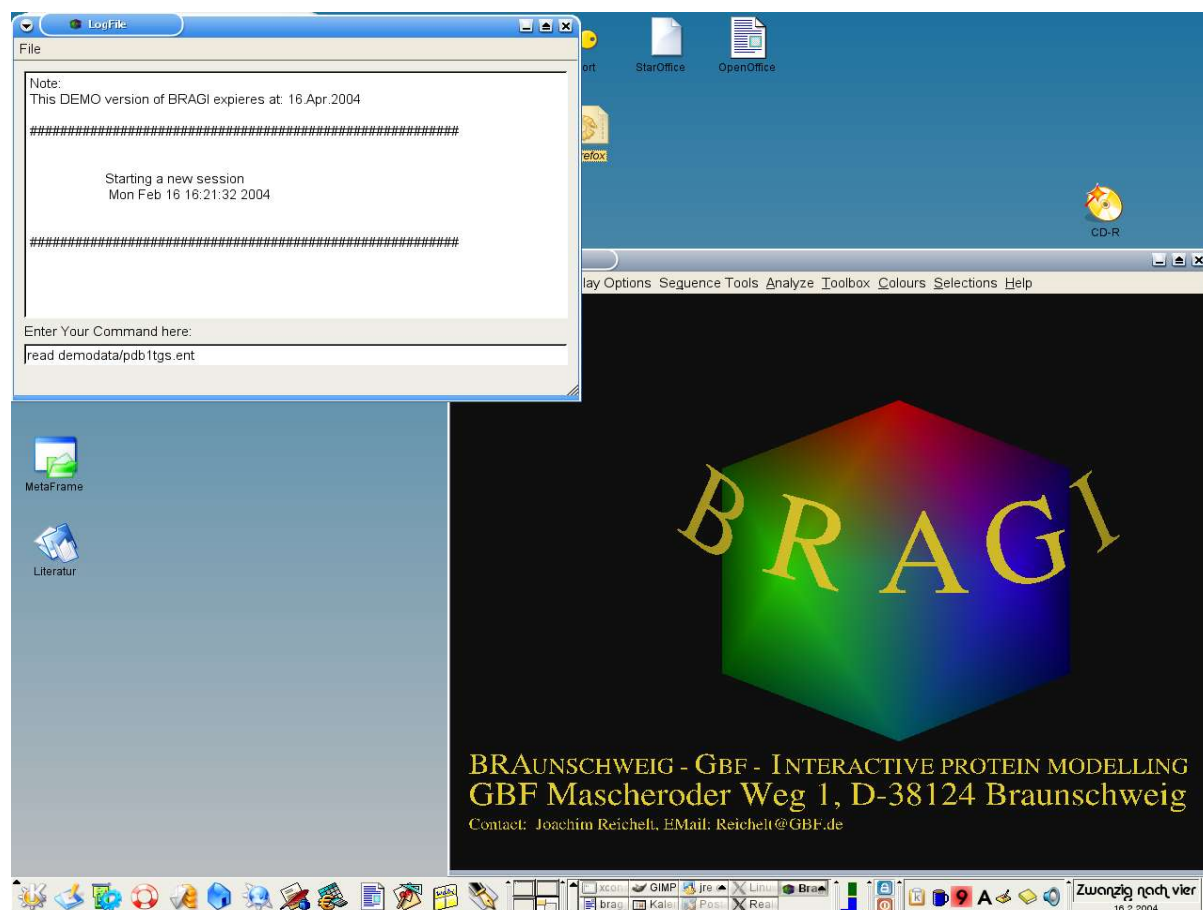
Making a shortcut from the file to your desktop easily does this.

To start BRAGI on Linux/Unix
use the script **StartBragi**.

How to begin your BRAGI session

BRAGI starts with two windows, the 3D graphics window with a menu bar and the log window with a command input line.

The main window looks like this, before reading in a structure:



The *LogFile* window shows many useful information. In the one line command line you may enter any command known to BRAGI. For known commands see the so called batch syntax, because command may be given in batch files too.

Visualization:

Rotation in BRAGI:

All rotations and translations are applied according to a **fixed** coordinate system where the "imaginary" coordinate system is located so that the positive x-axis points from the left side of the screen to the right side. The positive y-axis points up from the bottom of the screen and the positive z-axis points from the screen to your nose.

Pressing the **LEFT** mouse button and moving the mouse in the x-axis (right-left) direction rotates the object around the **y-axis**.

Pressing the **LEFT** mouse button and moving the mouse in the y-axis (up-down) direction rotates the object around the **x-axis**.

Pressing the **LEFT** mouse button and the **SHIFT** key together and moving the mouse in the y-axis (up-down) direction rotates the object around the **z-axis**.

Pressing the **control** key will allow fine adjustments.

If you are using a two button mouse press "R" to select rotation.

Translate a structure in BRAGI:

Pressing the **MIDDLE** mouse button and moving the mouse in the x-axis direction or moving the mouse in the y-axis direction translates the object in that direction.

Pressing the **MIDDLE** mouse button and the **SHIFT** key together and moving the mouse in the x-axis direction translates the object in the z-axis direction.

Pressing the **control** key will allow fine adjustments.

If you are using a two button mouse press "T" to select translation and use the **LEFT** mouse button.

Scaling:

Pressing the **RIGHT** mouse button and moving the mouse in the +x-axis or +y-axis direction zooms the object upwards and the -x-axis or -y-axis direction zooms the object downwards.

Slab:

Pressing the **RIGHT** mouse button and the **SHIFT** key together and moving the mouse in the +x-axis or +y-axis direction increases the slab thickness and the -x-axis or -y-axis direction decreases the slab thickness.

Pressing the **control** key will allow fine adjustments.

The coordinate system

BRAGI uses only one coordinate system where the center of the coordinate system is in the middle of the graphics screen. The positive x-axis is running to the right and the negative x-axis to the left. The positive y-axis is running upwards and the negative y-axis downwards. The Positive z-axis is running out of the screen and the negative z-axis into the screen.

All molecules are rotated and translated independent, but you may select any

number of molecules to be moved together. Default is to move all molecules.

The Menu bar

Many functions of BRAGI are controlled by pull down menus.

Functions not implemented are marked **green** some of them are hidden too.

FILE menu has these options:

- **Open:** Opens file for reading
 - **PDB Structure:** The files are split to different molecules by chain identifier by default
 - **PDB Structure (to One Molecule):** the structures is read in to one molecule, ignoring all information in the structure file as e.g. "TER"
 - **Get Coordinates from RCSB:** retrieve a structure directly from RCSB via ftp. All you have to know is the four letter code.
 - **MMCIF:** Structures in the mmCIF format
 - **Batch:** Command scripts
 - **Surface:** read a precalculated surface for one displayed structure
 - **H-Bonds:** Table of H bonds for one displayed structure
 - **Secondary structure:** read secondary structure information for one displayed structure
 - **NOE shifts:** read NOE shifts to calculate NMR spectra for one displayed structure (not jet working!)
 - **Electron transfer:** read electron transfer calculated by pathways for one displayed structure
 - **Transformation Matrix:** read the 4x4 translation and rotational matrix for displayed structures
- **Save:** Saves various things
 - **in PDB Format:** Write out a PDB formatted file of displayed structures
 - **Write in PDB Format at the &#amp;Original Positions:** Write out a PDB formatted file of displayed structures, ignoring all translations and rotations made by the user
 - **Coordinates and Charges (... Format):** Coordinates and additional charges are written to different types of the pseudo PDB file
 - **Coordinates and Charges (... Format) at the Original Positions:** Coordinates and additional charges are written to different types of the pseudo PDB file, ignoring all translations and rotations made by the user
 - **Biografs .bgf:** Write out coordinates in the format used by BIOGRAF and by pathways (to calculate electron transfer)
 - **Surface:**
 - **NOE Simulation** saves the NMR prediction (not yet functional)

- **Transformations:** Save the translation and rotation of one structure. These are kept separate for each structure in BRAGI.
- **Sequence:** The sequence is saved in an extended format (.psq). It may be easily converted to other formats.
- **Status:** The status is a dump of the state of BRAGI. It may be read in to a newly started BRAGI session before reading in molecules. The settings of BRAGI may be modified and saved as defaults for later sessions. This includes location of files or the width of lines
- **Screenshot:** A screenshot or hardcopy is a pixel by pixel dump of the main graphics saved to a file. These files are suited to be viewed with all newer browsers.
- **create a Movie:**
- **Open Recent:** shows the 10 recent files opened in BRAGI for fast rereading
- **Exit...:** Shut down program.

EDIT menu has the options:

- **Delete Molecule(s):** Opens a dialog to select the molecules to be deleted.
- **Create Molecule:** To create a new molecule.
 - **Create Protein:** the new molecule is build only of amino acids
 - **Create Nucleotide:** the new molecule is build only of nucleotides
- **Rotate Around Bonds:** opens a dialog to select or pick a residue. All known torsions may be adjusted using one dialog.
- **Exchange Residues:** opens a dialog to select or pick a residue. Then a dialog asks for the new residue type to replace it with.
- **Append Residue:** opens a dialog to select or pick a molecule. As many residues of the same kind - e.g. amino acids - may be appended as wanted.
- **Automatic Replacement:** opens a dialog to select or pick a molecule and an alignment file. BRAGI will replace the sidechains according to the alignment. No residues are removed from the start structure, instead residues, that should be deleted, are replaced by GLY. No new residues are inserted. Use Protein-Loop or Loop Prediction to get this done.
- **Copy:** Copies the selected residues to an internal buffer.
- **Cut:** Copies the selected residues to an internal buffer. Then these residues are deleted from the molecule.
- **Paste Before:** opens a dialog to select the molecule. The internal buffer is inserted between this residue and the one before it in the sequence.
- **Paste After:** opens a dialog to select the molecule. The internal buffer is inserted between this residue and the one following it in the sequence.
- **Paste to New:** Creates a new molecule of the internal buffer.
- **Protein-Loop:** opens a dialog to replace a sequence of residues by 3... 10 residues.
- **Loop Prediction:** opens a dialog to replace a sequence of residues by 3... 10 residues.
- **Remove water:** opens a dialog to select molecules. All solvent residues of these molecules are deleted.
- **Remove Heteroatom:** opens a dialog to select molecules. All hetero residues, e.g. cofactors and solvent of these molecules are deleted.

VIEW menu has a set of radio buttons (checked means show). The usage of these

buttons affects only visible marked molecules. So it is possible e.g. to show only the secondary structure of the third molecule by first switching off all molecules but the third. The switch on secondary structure and at the end to switch on all molecules.

- **Main Chain:** This are N, C, CA, O atoms of amino acids.
- **Hydrophob Groups** This are ALA, CYS, ILE, LEU, MET, PRO, and VAL
- **Hydrophil Groups** this are ASN, GLN, SER, and THR
- **Aromatic Groups** this are HIS, PHE, TRP, and TYR
- **Positively Charged Groups** this are ARG and LYS
- **Negatively Charged Groups** this are ASP and GLU
- **Show all above:** toggles all the 6 buttons on or off
- **Connectivities:**
- **Disulfide Bonds:**
- **Hetero Atoms:** this are all HETATM records, but not water molecules
- **Solvent:** this are the well know solvent molecules HOH, WAT, OHH, SOL
- **Secondary Structures:** this is the secondary structure as read in. Normally the related lines are included in a PDB file. But you may recalculate it.
- **Surface:**
- **CPK/Ball and Sticks:**
- **Labels:**
- **Hydrogen Bonds:** this are H bonds calculated by tools inside BRAGI
- **Non-bonded Contacts:** this are all interactions calculated by tools inside BRAGI

Display Options menu has the options:

- **Visible Secondary Structure:** Change image options for secondary structures.
- **Calculate CA-Tube:** Use it to define the tubes BRAGI will use to highlight the folding of a protein or nucleotide.
- **Center:** center at a selected atom
- **automatic Center and scale:** centers and scales the display to show all molecules.
- **Animate:** to animate the shown molecules by switching on and off sets of molecules, use this.
- **Roll:** BRAGI will rotate the movable molecules by 1° around the Y axes
- **CPK/Balls/Sticks:** This will open a dialog to show atoms as spheres and bonds as cylinders. The size of the spheres is .1 to 2 times their van der Waals radii. The diameter of the sticks is .1 to 1.0 Angstroms.
- **Show Line between Atoms:** to show interaction of two atoms you may add a stick or a line of balls from one atom to any other atom of the same molecule.
- **Free Text:** Text of any size can be used in BRAGI. This text may have a fixed position or moved with a molecule.
- **Marker:** Marker are lines, arrows, and rectangles, hollow or solid, of any size. This markers may have a fixed position or moved with a molecule.
- **Label:** are identifier of residues or atoms and are moved together with it.
- **Projective:** is the default display mode of BRAGI. Objects closer the viewer are larger then those in the background.
- **Stereo Zscreen:** BRAGI will try to use hardware stereo if available, if not BRAGI switches to full screen and shows a squeezed view. Use a frame doubler and appropriate glasses to get stereo view of your molecules.
- **Stereo Dual View:** Bragi switches to side by side stereo. There is a known method, to get hardware alike stereo using this option. See

<http://netjuggler.sourceforge.net/SoftGenLock.php> for more information.

- **Screenshot:** Just make a digital image of what you see in the main graphics.
- **Ray Tracing:** Solids, e.g. spheres, sticks, and tubes are transferred to a file, povray can interpret. See <http://www.povray.org/> for more information
- **Create VRML-File:** Solids, e.g. spheres, sticks, and tubes are transferred to a VRML file. This may be viewed using any VRML enabled browser or software.
- **Options:** Use this to set and reset to its initial values various options of the display, the scale, stereo separation, thickness of the visible volume, text height and quality, line smoothing depth cueing. Additionally you may translate and rotate the molecules by specified values. Instead of rotating around the X and Y axes you may switch to a virtual trackball.

Sequence Tools menu has the options:

- **Show Sequence:** will show the sequence of selected molecules. Helices, Beta sheets and Turns are color coded. You may select residues and mark these in the graphics.
- **SWISSPROT:** tries to get all known information from SWISSPROT on a PDB structure. This feature heavily depends on the name of the molecule, as given in the HEADER line of the PDB file.
- **InterPro:** tries to get all known information from InterPro on a PDB structure. This feature heavily depends on the name of the molecule, as given in the HEADER line of the PDB file.
- **Human Mutation Databases:** tries to get all known information mutations of a PDB structure. This feature heavily depends on the name of the molecule, as given in the HEADER line of the PDB file.
- **Blast search:** Will trigger a real search on the blast server with the sequence of the selected molecule.

Analyze menu has the options:

- **Show brief Information:** Shows all known information on one or more molecules: The source file, its Compound name, Source, Author(s), a count of amino acids, the estimated mass and volume.
- **Show Hierarchy Window:** shows a hierarchical view of the molecules. This view is used the same way as a file view. Click on a + to expand a subtree, - to collapse it. A lot of useful information is shown in this view. Use it to select regions or to search for additional information not visible in the graphics most of the time.
- **Show full Information for PDB entry:** will popup a browser window, to retrieve all information stored in the PDB file in human readable form and additional links. This feature heavily depends on the name of the molecule, as given in the HEADER line of the PDB file.
- **Distances/Angles:** pops up a dialog to select up to 4 atoms. BRAGI will try to calculate all distances, angles, and the dihedral. The result may be transferred to the main graphics, to highlight special geometry.
- **Bonds/H-Bonds:** pops up a dialog to select a range of residues. Interactions of this range with another range of residues or with other molecules are calculated. Then the list of found "bonds" is shown for further usage.
- **Distances around one atom:**
- **(Phi, Psi) Search:**
- **Analyze and check residue:** Select a residue in the dialog to get geometric

information on it.

- **Search for Domains.** BRAGI will try to identify structural domains of the selected region of a molecule. This range must consist only of amino acids.
- **Calculate Secondary Structure:** The secondary structure for selected molecules is calculated based on the publication of Kabsch and Sander, 1988
- **Regions of Interest:** Select a residue or atom. BRAGI will show only residues based on the distance to the selected object.
 - Show only objects inside a sphere of ... Angstroms
 - Show also objects inside a sphere of ... Angstroms
 - Show all objects outside a sphere of ... Angstroms
 - Show all (again)
- **RMS Deviation:**
- **Automatic Protein Fitting:**
- **Semiautomatic Protein Fitting:**
- **PHI/PSI Deviation:**
- **Ramachandran Plot:** This will create a Ramachandran plot of one or more Molecules. A Ramachandran plot is a X/Y plot of the backbone dihedrals PHI and PSI. Clicking with the left mouse button on a letter, click a second time will add a small window at the cursor position showing the identification of this residue and the backbone torsion angles. This window may be moved using the middle mouse button and deleted using the right mouse button.

Toolbox menu has the options

- **Create Topology:** BRAGI is using known information on residues, e.g. connectivities, masses, etc. But sometimes these informations are wrong due to the usage of other names as used in BRAGI. You may select a residue. BRAGI will try to recalculate the connectivities based on distances. You may want to save this information for further processing.
- **Secondary Structure:** The secondary structure for selected molecules is calculated based on the publication of Kabsch and Sander, 1988
- **Calculate Surface:** BRAGI knows different types of surfaces. All of them are calculated by external programs. We supply two programs to calculate a nice smooth color coded too solid surface, and a fast program to calculate solid or wireframe surfaces, that are color coded too. The later program can calculate surfaces clipped to a sphere or a cube.
- **Apply Symmetry Operation:**
- **Build unit cell or monolayer:**
- **Add and optimize polar hydrogens:**
- **Add all known hydrogens:**
- **Set/delete Bonds:**
- **Check bondlength:**
- **Calculate NOE simulation:**
- **Solvate molecule(s):**

Colours menu has the options:

- **Colour by Molecule:** All atoms are shown in the colour of the backbone
- **Colour by Group:** This is the usual default in BRAGI. The colour code used here is based on physical properties.
- **Colour by Atom:** All atoms are shown in colours used in chemistry.

- **Colour by Temperature Factor:** If there were temperature factors in the PDB file, BRAGI will assign the atoms to groups representing their temperature factor. The colours of this molecule will be changed to show atoms with high temperature factor in red, with low temperature factor in blue.
- **Colour by Occupancy:** If there were occupancies in the PDB file, BRAGI will assign the atoms to groups representing their occupancies. The colours of this molecule will be changed to show atoms with low occupancies in red, with high occupancies in blue.
- **Colour by accessible surface:** the more part of the surface of an individual residue is accessible, the colour will change from blue to red
- **Assign to another Colour Group:** Here you may modify the assignment of residues to the colour groups.
- **Colour Change:** This does what you expects. It pops up a dialog to adjust nearly any colour used in BRAGI.
- **MD Colours:** Colour code is related to properties of an molecular dynamics run
- **Adjust Surface Colours** If BRAGI has any knowledge on the vertices of a surface, BRAGI can change the colour code of the surface.

Selections menu has the options:

- **Pick Residues:** If you pick an object, whole residues are selected
- **Pick Atoms:** if you pick an object, atoms are selected
- **Select visible Molecules:** Molecules may be hidden. This does not affect the movement of it!
- **Select active Molecules:** Molecules may be excluded from rotation and translation. This does not affect the visibility!

HELP menu has the options:

- **manual:** show manual, at now in acrobat reader.
- **Settings:** opens a dialog to set a lot of parameters used by BRAGI, e.g. locations of files, display option, URLs to retrieve data etc.
- **About:** show information about BRAGI, e.g. copyright, version...

The Popup menu

Some often used functions are accessible by popup menus.

TO get a popup menu press the right mouse button.

The popup menu of the main graphics:

- **Selection mode**
 - **Atom:** If you pick an object, atoms are selected
 - **Residue:** If you pick an object, whole residues are selected
 - **Molecule:** If you pick an object, whole molecules are selected
- **Expand selection to residues:** all those residues are selected, whenever at least one atom is selected
- **Expand selection to molecules:** all those molecules are selected, whenever at

- least one atom is selected
- **Set**
 - **set Sticks**: All connections of two selected atoms are drawn as sticks
 - **set CPK**: All atoms are drawn as spheres
 - **set Ball and Stick**: All connections of two selected atoms are drawn as sticks, all atoms are drawn as spheres
 - **set Label**: Depending on the selection mode, all selected atoms or all selected residues are labeled.
 - **Remove**
 - **remove Sticks**: All sticks of two selected atoms are removed
 - **remove CPK**: The selected atoms are no longer drawn as spheres
 - **remove CPK, Ball and Stick...**: All sticks of two selected atoms are removed, the selected atoms are no longer drawn as spheres
 - **remove Label**: Depending on the selection mode, labels of all selected atoms or all selected residues are removed.
 - **remove selection**: the selection is copied to the internal selection buffer and removed from the molecule. There should be only one continuous region of selected residues.
 - **Center here**: All molecules are shifted to center the selected atom to the display. If more than one atom is selected, BRAGI calculates a regular box surrounding all these atoms and will center this box.
 - **unselect all**: All atoms are unselected.

Selection

Several functions in BRAGI allow the usage of selection in the same way as done in e.g. word processors.

There are different ways to select objects in BRAGI:

- **Picking**
 - double click on any atom to select this. If the selection mode is residue, the whole residue is selected, if the selection mode is molecule, the whole molecule is selected.
 - If you press the CTRL button, while clicking, this object is selected additional to the existing selection.
 - If you press the SHIFT button, while clicking, all residues between the last selection and this selection are selected, even when your selection mode is atom.
- **Using the Tree View**

Using the pulldown menu Analyze, then Tree View, you get a view off all objects, you may select. In this view, selection is done in the following way:

Expand the tree view by clicking on the + sign, if needed.

 - Click on an Molecule, residue or atom to select it. Hidden objects are selected automatically.
 - Press the left mouse button while moving over several objects will select all of them
 - Use the CTRL button to add objects to the selections

- Use the SHIFT button to select a range of objects

Some dialogs will set selections to.

Utility programs:

All these executable programs are located in subdirectories of the Tools-directory.

For direct usage:

amb2bragi

Converts an AMBER prep file into a BRAGI topologie file.

Csd2bragi

Converts an AMBER prep file into a BRAGI topologie file.

bragi2amb

Converts BRAGI topologie file into a an AMBER prep file. This is obsolete due to antechamber of AMBER 7.0.

homol

Sequence alignment program based on ideas of Prof. Schomburg.

gbfssp

Program to calculate secondary structures.

Internal helpers for BRAGI:

surface

Internal program to calculate solid and wire frame surfaces.

predictor4bragi

Loop prediction program.

deep

automaticreplacement of sidechains

The batch syntax used by BRAGI

How to define objects:

Definitions:

- [] stands for options and may be given or not
- <> stands for options that must be present
- * is a wildcard
- | separate alternatives of options. Exact one of them has to be present
- Defaults are written underlined
- Options are separated by spaces

To define range of objects use:

Moleculename;ChainId;First residue; Second residue; [List of Atomnames];

Do not forget any of the semicolons. There must be 6 of them!

Additionally we allow a long format:

[Mol] <Moleculename> [Chain <ChainId>] [Residue <First residue> [- <Second residue>]] [Atoms <List of Atomnames>]

To define a single object use:

Moleculename; ChainId; Residue; [Atom];

Do not forget any of the semicolons. There must be 4 of them!

Additionally we allow a long format:

[Mol] <Moleculename> [Chain <ChainId>] [Residue <Residue >] [Atom <Atomname>]

Examples on how to select regions or sets of residues

- Enter the full name, including insert code if appropriate
 - ARG 14 exactly matched
 - HIS 195B exactly matched
- Use wildcards
 - * 14 all residues with the given number 14, or the first found, if only one residue is allowed
 - 14 the 14th residue of the selected chain, its number or name does not matter
 - FIRST the first residue of the selected chain
 - LAST the last residue of the selected chain

How to select regions or sets of residues and atoms

- Enter a list of atom names. Wildcards are not permitted. Separate the elements by commas. Giving more than one atom where only one is allowed, is an error

Examples:

1_5pti ; ; 1; 12; C, CA, N, O;

Here all atoms with name „C“, „CA“, „N“ oder „O“ of the residues from 1 to 12 of the molecule named 1_5pti are selected

Mol 1_1tgs Chain Z Residue *1 - *12 Atoms CA, CB

Here all atoms with name „CA“ oder „CB“ of the residues starting at the one with the given number 1 and ending at the one with the given number 12 of the molecule named 1_1tgsi are selected.

It is shorter to write:

1tgs; Z; *1-*12; CA,CB;

If a command uses only one object, e.g. one residue or atom:

1_5pti ; ;ILE 16; C;

Alphabetical list of known commands

| <i>Command</i> | <i>Function</i> |
|----------------|---|
| # | Comment, remainder of the line will be “echoed” |
| ; | Comment, remainder of the line will be “echoed” |
| @ | Call a new Macro file, see CALL |
| ANGLE | Calculates the angle of 3 atoms |
| ANGLES | Calculates the angle of 3 atoms, see ANGLE |
| APPEND | Append residues |
| ASSIGN | Assign residues to color groups |
| BALLLINE | Connect two atoms by a line of balls or a cylinder |
| BUILD | Create new Molecules, cf. APPEND |
| CALL | Call a new Macro file |
| CENTER | Center the graphics at |
| COLOR | Changes the color |
| COLORMODE | Set the colors of this Molecule to a predefined mode |
| COLOUR | See COLOR |
| COLOURMODE | See COLORMODE |
| CONNECT | Check for bonds and H-bonds |
| CONNECTS | See CONNECT |
| CPK | Display atoms as spheres |
| CUT | Move a region of residues to a private buffer |
| DELETE | Remove molecules |
| DESELECT | Remove these objects from the selection list |
| DIEDER | Calculates the dihedral angle of 4 atoms |
| DISTANCE | Calculates the distance of 2 atoms |
| DRAW | (Un)Sets creation of hardcopies for every shown frame |

| <i>Command</i> | <i>Function</i> |
|----------------|--|
| END | Ends torsion, ends batch script |
| EXCHANGE | Replace a sidechain by another |
| EXIT | End of (this) macros |
| FIX | Do not move selected molecules |
| FOG | Set the fog for different objects |
| HARDCOPY | Make a screen dump |
| HIDE | Undisplay selected molecules |
| LABEL | Place a label at selected position |
| MARKER | Set and remove markers, e.g. arrows |
| MOVE | Do move selected molecules |
| NEIGHBORS | Calculates all atoms in a sphere around a given atom |
| NEIGHBOURS | See NEIGHBORS |
| NOVERBOSE | Command lines are no longer echoed |
| OFF | Undisplay selected molecules. See HIDE |
| ON | Display selected molecules. See SHOW |
| OPEN | Read in a file. See |
| OPTION | Sets options for reading structures |
| OPTIONS | See OPTION |
| PLOT | See HARDCOPY |
| POVRAY | Start raytracer |
| PROFIT | Automatic fitting of proteins |
| RAMACHANDRAN | Creates a Ramachandran graph |
| RAYTRACER | Start raytracer |
| READ | Read in a file. See OPEN |
| REM | comment, remainder of the line will be "echoed" |
| REPEAT | Repeat the following command |
| RMS | Fitting of proteins |
| ROTATE | Rotates active molecules |
| SAVE | Writes out a PDB file. See WRITE |
| SCALE | Scales all molecules |
| SELECT | Add these objects to the selection. It does not unselect the old selection |
| SETUP | Setup torsion mode |
| SHOW | Do not hide selected objects |

| <i>Command</i> | <i>Function</i> |
|-----------------|---|
| SLAB | Set the slab size |
| SLEEP | Sleep for <seconds> seconds |
| STICK | Displays bond as cylinders |
| STOP | Stop this script here, remainder of file is ignored |
| SURFACE | Reads in a precalculated surface |
| TORSION | Performs a dihedral torsion, see SETUP to setup this mode |
| TORSIONRELATIVE | Performs a dihedral torsion, see SETUP to setup this mode |
| TRANSLATE | Translate all molecules |
| WRITE | Writes out a PDB file |
| VERBOSE | All commands are echoed |

Explanation of the batch syntax used by BRAGI

All these commands may be given in the command line of the “LogFile” window too

Text marked in green are at now not accessible by batch scripts. You have to use the normal user interface.

The order of the commands is based roughly on the order of the menu.

Read in coordinates:

OPEN | READ [Brookhaven | MMCIFF] < filename >

Set the Options before reading with

OPTION READ <CHECK <ON|OFF>> <SEPERATE<ON|OFF>>

Get Coordinates From RCSB

OPEN | READ RCSB <4 Letter Code>

Read in a precalculated surface:

OPEN | READ SURFACE < filename > [options]

the options are:

COLO[U]R < Molecule | Electrostatic | Hydrophility >

LINETYPE <DOTS_AT_VERTICALS | SOLID | DASH DOT|

DASH_DOT | DASH_DOT_DOT | LONG |CENTER_DASH |

CENTER_DASH_DASH | LONG_DASH_DOT | VERY_LONG >

Linetype is ignored, if reading in a solid surface.

Read in a precalculated H-Bonds:

OPEN | READ HBONDS < filename >

Read in a precalculated Secondary Structure:

OPEN | READ SECSTRUCT < filename > <molecule>

Read in a precalculated NOE-Shifts:

OPEN | READ NOE < filename > <molecule>

Read in precalculated Electron Transfers, calculated by “pathway2”:

OPEN | READ ELECTRONTRANSFER

< filename > [<molecule> [<molecule> [...]]]

BRAGI tries to match the values to the given molecules

Read in a Transformation Matrix:

OPEN | READ MATRIX < filename > [<molecule> [<molecule> [...]]]

If molecule is omitted, ALL molecules will get this matrix, as if they were all moved together.

Call another script:

CALL | @ < filename >

Stop a batch script

STOP

This will stop the usage of this batch script, ignoring the remaining part of it.
This is mainly for debugging

Save coordinates, Charges, Surface, Transformation Matrix, Sequence, Status or Settings:

WRITE| SAVE <Keyword> < filename > [< list of molecules >]

Keywords are:

BROOKHAVEN (may be omitted, is default)
BROOKHAVEN_UNMOVED
MMCIF
BROOKHAVEN_GRASP
BROOKHAVEN_GRASP_UNMOVED
BROOKHAVEN_AUTODOCK
BROOKHAVEN_AUTODOCK
BIOGRAF
SURFACE
NOE
TRANSFORMATION
SEQUENCE
STATUS
SETTINGS

Dump the graphigs to a file:

HARDCOPY

[<[CREATE [basename [extension [Number]]]] | [Name]>]

Defaults are:

Name: Bragi-hardcopy
basename: BRAGI_HARDCOPY_
extension: ppm
Number: Start with 0, increment the last by one.

Immediately exit BRAGI:

EXIT

the options are:

FORCE do not ask for confirmation

Delete one or more molecules:

DELETE < list of molecules | * (=> all molecules) >

Append residues to an existing molecule or build a new molecule:

APPEND| BUILD < molecule name > < @ < filename > | list >

use this syntax for the list:

[CONFORM < Rightalpha | Leftalpha | parallel | antibeta |
[specific] <phi> <psi> <omega> >]
[LAMINO | DAMINO]
[HYDROGEN < None | Polar | Charged | NOE | All >]

[SEQUENCE] < list of residue names, use 3 letter code >)

BUILD will always create a new molecule, APPEND append residues to an existing molecule.

Using the option '@ <filename>' all residues are read from a file. The format of each line has to be:

< Previous | residue name > <phi> <psi> <omega>

The keyword 'Previous' is allowed only in the first line, it sets Psi and Omega.

Psi and Omega are the dihedrals to the next residue, so we have to know them to append the first residues. For omega use the shorts: t is trans, c is cis):

Example

```
Previous 113 t
ALA -119 113 180
ARG 57 47 c
TRP 136 113 180
ARG -119 113 0
```

...

Change known dihedral. Note there cannot be more the one torsion active at a time!
Select the residue

SETUP TORSION <residue>

Change dihedrals

TORSION <dieder name> <value>

TORSIONRELATIVE <dieder name> <change>

Finish torsion mode

END TORSION

Replace a sidechain

EXCHANGE <residue> <new name>

Copy a range of residues to the clipboard and remove it from the old molecule

CUT <residue range>

Copy a range of residues to the clipboard

COPY <residue range>

Copy a range of residues from the clipboard

PASTE < NEW | AFTER <residue> | BEFOR <residue> >

Copy the residues from the clipboard to a new molecule or insert them into an existing one

It does not make sense to implement the highly interactive topics in a batch system:
Protein Loop, Loop Prediction

Remove all Water (-molecules)

REMOVE_WATER [< molecule [< molecule [...] >] >]

Remove all so called Heteroatoms (HETATM records)

REMOVE_HET [< molecule [< molecule [...] >] >]

Switch on or of parts of the molecule by color code

SHOW | ON < Mainchain | Hydrophob | Hydrophil | Aromatic | Positive | Negative | Connect | Ssbond | Hetero | Solvent | SecStructure | Surface | Label | Cpk | Line | Ribbon | Helix | Helix Cylinder | Helix Ribbon | Sheet | Turn >

HIDE | OFF < Mainchain | Hydrophob | Hydrophil | Aromatic | Positive | Negative | Connect | Ssbond | Hetero | Solvent | SecStructure | Surface | Label | Cpk | Line | Ribbon | Helix | Helix Cylinder | Helix Ribbon | Sheet | Turn >

Select visible secondary structure elements

VISIBLE_SEC

Options are:

ON | OFF
BETA <ON | OFF >
CA_LINE <ON | OFF >
CA_RIBBON <ON | OFF >
CA_TUBE <ON | OFF >
HELIX_CYLINDER <ON | OFF >
HELIX_RIBBON <ON | OFF >

Calculate CA-Tubes

Calculate Tubes showing the C α trace

CA_TUBES < option(s)> <range>

Options

SCHMA <RESIDUE|HYDROPHIBICITY|CALPHA| SECONDARY|
SINGLE| TEMP_FACT|TEMP_FAC_COL>
AXIS< X Y > [COLOR < Color>]
HELIX < X Y > [COLOR < Color>]
BETA < X Y > [COLOR < Color>]
TURN < X Y > [COLOR < Color>]

Using multiple options, the last one will overwrite previous. Default is "SCHEMA SECONDARY"

Center the display to a given atom:

CENTER < Atom >

Translate all displayed molecules

TRANSLATE [X <X value>] [Y <Y value>] [Z <Z value>]
values are in Angstroms

Rotate all displayed molecules

ROTATE [X <X value>] [Y <Y value>] [Z <Z value>]
values are in deg, 360 is a full rotation

Scale all molecules

SCALE <value | ABSOLUTE <value> >

Animate, Roll

Set or delete CPK's (Spheres):

CPK [options] [<region of residues and atoms>]

options are

[On | Off]

[Radius <relative to the Van-der-Waals radius, default: 1.0>]

[Backbone | CAlpha | All]

[Colour (< red > <green > < blue >) | Multicolorur]

Default is: ON, All selected residues

Set or delete Sticks:

STICK [options] <region of residues and atoms>

Options are the same as for CPK, but
radius is in Angstrom
default radius is 0.2.

Connect two atoms by a line of balls

BALLLINE <radius> <red> <green> <blue> [COUNT n] <Atom from> <Atom to>

This will draw n Balls on the straight line between these atoms. Default for n is 7.

Manage free form text

TEXT

Options are (use this order!)

AT < X, Y, Z>

COLOR <color name>

SIZE <Angstrom>

BOUNDTO <molecule|BACKGROUND>

Text

or

DELETE <Number>

You must not omit any option at all, there are no defaults. Do not change the order of the options!

The numbers are given at creation time, starting at "1", so at now you have to count yourself.

Place Markers:

MARKER [options]

Options are (use this order!)

< TYPE < SOLIDARROW | SOLIDBAR | ARROW | BAR | LINE |
DASHEDLINE | DOTTEDLINE | DASHDOTLINE | DASHDOTDOTLINE

| BALLS <count> >
FROM <X> <Y> <Z> TO <X> <Y> <Z>
COLOR <color name>
WIDTH < Angstrom>
BOUNDTO <molecule>

or:

DELETE <Number>

You must not omit any option at all, there are no defaults. Do not change the order of the options!

The numbers are given at creation time, starting at "1", so at now you have to count yourself.

Set or delete Label:

LABEL [ON | OFF] [< Residue> | <Atom>] <region of residues and atoms>
Default is: ON, All selected residues

Set the display mode to and from stereo

VIEWMODE

Options are:

PROJECTIVE
HW_STEREO
Z_SCREEN
SIDE_BY_SIDE

BRAGI will try to switch to the desired mode, even if it is not really possible.
Results may vary depending on your hardware

Prepare or start Raytracing:

POVRAY

Options:

[FILE] <Name>
CALCULATE
DISPLAY
WIDTH <value>
HEIGHT <value>
OPTS < List of keyword for raytracer>

Prepare a VRML file

VRML <filename>

BRAGI will try to write out all displayed object in the VRML format for use with VRML enabled browsers

[ShowSequence](#), [SwissProtGroup](#), [InterProGroup](#), [OmimGroup](#), [CluSTr](#), [Blast](#)
[ShowInformation](#), [ShowTree](#), [ShowMoreInformation](#)

Calculate distance of two Atoms

DISTANCE <Atom from> <Atom to>

Calculate angle of three Atoms

ANLGLE <Atom1> <Atom2> <Atom3>

Calculate the dihedral build by four atoms

DIEDER <Atom1> <Atom2> <Atom3> <Atom4>

There is no need for this 3 commands, to select connected atoms.

The result is displayed in the graphic by green lines.

Highlight distances to atoms in a sphere around another atoms

NEIGHBORS <atom> [INTERMOLECULAR] <maxDistance>

This will draw lines to all atoms that are close <maxDistance> to this atom.

Default is to check only the molecule this atom belongs to

(Phi, Psi) Search, Analyze and check a residue, Search for Domains, Calculate Secondary Structure

Calculate possible bonds, contacts, and H-Bonds

Check for intermolecular bonds:

CONNECT MOLECULE < molecule name > CHECK < covalent | Hbonds >
[options]

Options are:

[INTRA] [INTER < list of molecules >]
[TYPE < Protein, Nucleotide, Sugar, Solvent, Other, All >]
[IGNOREPROTOP] [IGNORETOP]
[SIGMA <tolerances of distances>]

Check for bonds of residues

CONNECT RESIDUE < residue range > CHECK < covalent | Hbonds > [options]

Options are:

[INTRA | INTER[WITH] <list of molecules> | WITH[RESIDUES] <residue range>]
[TYPE < Protein, Nucleotide, Sugar, Solvent, Other, All >]
[IGNOREPROTOP] [IGNORETOP]
[INTERNAL | NOINTERNAL]
[SIGMA <tolerances of distances>]

Fit two molecules or parts thereof:

RMS ((PAIR | FIT) <residue range> <start residue >) [OPTIONS < options >]

Options are:

[PROTEIN < all | mainchain | Calpha | ignore >]
[NUCLEOTIDE < all | backbone | ignore >]
[SUGAR < all | ignore >]
[OTHER < all | ignore >]
[INVERS]
[(SCALE < automatic | fixed <Maximum> >) | NoPlot | None]
[WITH <List of molecules to be moved too>]

Automatic Fit of two molecules:

PROFIT <residue range 1 > <residue range 2 > [options]

All options of 'RMS' may be used and additionally

[PRINT]

[MOVE]

SemiautomaticProteinFitting, PHIPSIDeviation

Show a Ramachandran Graph

RAMACHANDRAN <molecule>

Create Topology, Secondary Structure, Calculate Surface, Set/Delete Bonds, Check Bondlength, Calculate NOE Simulation, Solvate Molecule

Change the coloring schema for molecules

COLO[U]RMODE < Group | Atom | Temp[eraturfactor] | Occupancy > <
list of molecules >

Change the coloring schema for individual residues or atoms

ASSIGN < Mainchain | Hydrophob | Hydrophil | Aromatic | Positive | Negative
| Invisible | Visible >
[(Sidechain | Mainchain | Backbone) < region of residues > |
All <region of residues and atoms >]

Change the shown color

COLO[U]R < Backbone | Nonpolar | Hydrophob | Polar | Hydrophil | Aromatic
| Positive | Negative | Connectiv[ies|y] | Ssbond | label[s] | Ribbonn[s] | Helix |
Trace | Background >
< red > < green > < blue >
< list of molecules (Not for: 'Background') >

Adjust Surface Colours

Select molecules to be movable

MOVE <ALL | <List of molecules>

or not movable

FIX < All | list of molecules >

Freeze the display:

SLEEP < Seconds >

Bragi will "sleep" for this time, so there is no redraw of the scene at all!

Save each picture to a file

DRAW [options]

Options is one of:

HARDCOPY creates a *.ppm -File for each frame displayed,

Use it to create movies using e.g. mpeg_encoder

NO_HARDCOPY stops the creation of hardcopies

RAYTRACE creates a PovRay input file for each frame displayed to
create movies

NO_RAYTRACE stops the creation of povray files

Adjust darkening of displayed objects

FOG

Options are:

[<OFF|ON [<value>]>]
[TEXT<OFF|ON [<value>]>]
[STEREO<OFF|ON [<value>]>]
[CPK<OFF|ON [<value>]>]
[LINEAR] [EXPONENTIAL] [EXPONENTIAL2]

Repeat on command several times

REPEAT <count> <Command>

Command may be any command of this list.

Add objects to the selection

SELECT <ALL | <range of residues>

Some commands use the selected atoms or residues if no list was given.

Remove objects from the selection

DESELECT <ALL | <range of residues>

List of all Keyboard shortcuts

Keys to access menus and to perform simple graphical operations

| <i>Key</i> | | <i>Ctrl or Alt or Shift-Alt</i> | <i>Shift</i> |
|------------|-------------------------------|---|--------------------------------------|
| F1 | Help | CPK Dialog | Label Dialog |
| F2 | Options | Select visible Molecules | Select active Molecules |
| F3 | Save Brookhaven | Write Sequence | Save Surface |
| F4 | Read | Read Secondary Structure | Read Surface |
| F5 | Screendump | Read Batch File | Call Raytracer |
| F6 | Exchange residue | Rotate bonds | Loop prediction |
| F7 | Ramachandran graph | RMS fit | Protein fit |
| F8 | Reset form stereo | Stereo dual view | Hardware Stereo or Stereo top/bottom |
| F9 | Colour change | Distance measurement | Assign to colour groups |
| F10 | CPK | Calculate secondary structure | Search Bonds |
| F11 | Read Batch File | | |
| F12 | Calculate secondary structure | | |
| -> | Rotate Y | Shift X | Big Shift X |
| <- | Rotate -Y | Shift -X | Big Shift -X |
| ^ | Rotate X | Shift Y | Big Shift Y |
| V | Rotate -X | Shift -Y | Big Shift -Y |
| Page up | Rotate Z | Shift Z | Big Shift Z |
| Page down | Rotate -Z | Shift -Z | Big Shift -Z |
| Keypad + | Zoom in | Increase text size | Increase slab |
| Keypad - | Zoom out | Decrease text size | Decrease slab |
| Insert | Increase slab | | |
| Delete | Decrease slab | | |
| Backspace | Remove selection | | |
| Print | screendump | | |

Keys to toggle display of objects and to perform simple tasks

| Key | | Shift | Ctrl | Alt |
|--------------------|--|-------------------|-------------------|--------------------|
| 1...0 ¹ | Toggle Mol 1..10 | Toggle Mol 41..50 | Toggle Mol 11..20 | Toggle Mol 21..30 |
| A | Aromatic toggle | Aromatic on | | Aromatic off |
| B | Nonbond toggle | Nonbond on | | Nonbond off |
| C | Connect toggle | Connect on | Copy | Connect off |
| D | Disulfid toggle | Disulfid on | | Disulfid off |
| E | Secondary toggle | Secondary on | | Secondary off |
| F | | | | |
| G | | | | |
| H | Hetreo toggle | Hetreo on | | Hetreo off |
| I | Hydrophil toggle | Hydrophil on | | Hydrophil off |
| J | | | | |
| K | CPK toggle | CPK on | | CPK off |
| L | Lables toggle | Lables on | | Lables off |
| M | Mainchain toggle | Mainchain on | | Mainchain off |
| N | Negative toggle | Negative on | | Negative off |
| O | Hydrophob toggle | Hydrophob on | | Hydrophob off |
| P | Positive toggle | Positive on | | Positive off |
| Q | | | Quit ² | |
| R | Left mouse button is used to rotate molecule (default) | | | |
| S | Solvent toggle | Solvent on | Save | Solvent off |
| T | Left mouse button is used to translate molecule | | | |
| U | Surface toggle | Surface on | | Surface off |
| V | | | Paste to new | |
| W | | | | |
| X | Exit ³ | | Cut | |
| Y | Hydrogen-Bonds toggle | Hydrogen-Bonds on | | Hydrogen-Bonds off |
| Z | | | | |

¹ Use „0“ for molecule 10, to use normal counting method!

² Quit will stop BRAGI without any further confirmation

³ Exit will open a confirmation dialog to end the BRAGI session

How to access molecules by key combinations

| <i>Molecule</i> | <i>Press</i> |
|--|---------------------------------|
| 1, 2, 3, 4, 5, 6, 7, 8, 9, 10 | Number Key |
| 11, 12, 13, 14, 15, 16, 17, 18, 19, 20 | Number Key + CTRL |
| 21, 22, 23, 24, 25, 26, 27, 28, 29, 30 | Number Key + ALT |
| 31, 32, 33, 34, 35, 36, 37, 38, 39, 40 | Number Key + CTRL + ALT |
| 41, 42, 43, 44, 45, 46, 47, 48, 49, 50 | Number Key + SHIFT |
| 51, 52, 53, 54, 55, 56, 57, 58, 59, 60 | Number Key + CTRL + SHIFT |
| 61, 62, 63, 64, 65, 66, 67, 68, 69, 70 | Number Key + ALT + SHIFT |
| 71, 72, 73, 74, 75, 76, 77, 78, 79, 80 | Number Key + CTRL + ALT + SHIFT |

So use these rules:

- The number key is the base, use key "0" to toggle molecule 10, 20, 30, 40, 50, 60, 70, and 80
- Add 10 for CTRL
- Add 20 for ALT
- Add 40 for SHIFT