

Support for Maps in RasMol

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Introduction

Electron density maps are important in structural biology. Display of a map superimposed on a molecular model is an important technique in understanding how well the model agrees with the data. Maps tend to be large files that, until recently, had to be handled section-by-section or brick-by-brick to make them more manageable.

RasMol is a popular molecular graphics program, but it lacks support for display of electron density maps. In the past, this omission was a necessary consequence of the need to keep RasMol sufficiently "light weight" to allow it to run efficiently on small computers with limited memory. Many low-end computers now have enough memory to handle large maps.

Extensions to the RasMol command language are needed to support maps. DINO [9], CCP4MG [5] and PyMOL [2] provide

good models for how to superimpose externally loaded maps onto macromolecular structures in real time. The Structural Biology Extensible Visualization Scripting Language (SBEVSL)[1] provides a framework within which an overall scripting language is being created and which is being used as a basis for the new commands for RasMol.

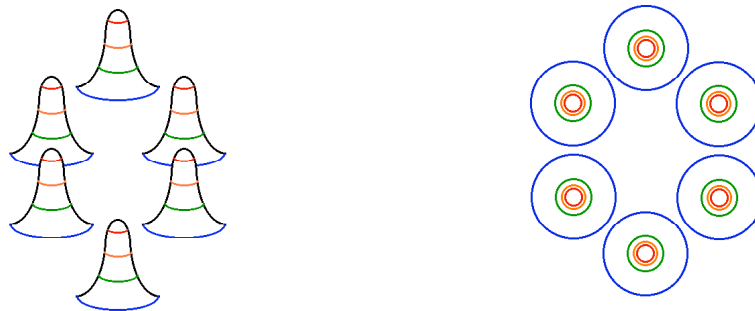
CCP4 map format has long been a de-facto community standard for map formats. imgCIF/CBF has recently been extended from handling 2D synchrotron images to also handling 3D images such as maps. Compression is important in handling large files, such as maps, but care is needed to avoid having to decompress the same data repeatedly.

We are using imgCIF/CBF compressed map support in the context of the SBEVSL scripting language to add map support to RasMol.

Electron Density Map Basics

“Electron density is the measure of the probability of an electron being present at a specific location. In molecules, regions of electron density are usually found around the atom, and its bonds...”

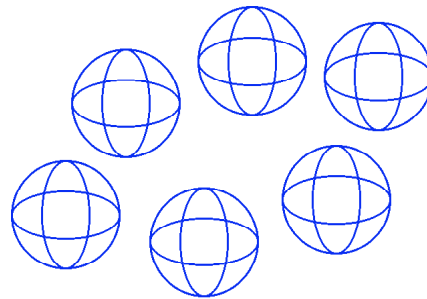
“To recover the electron density from [a] diffraction pattern by inverse Fourier transform, both amplitudes and phases are needed. Experimentally usually only the amplitudes can be measured...”



“Electron densities may be displayed in either one of two different styles: the first (and commonly used) style is with

electron density contours, the second style is electron density isosurfaces [mesh or transparent].” [6]

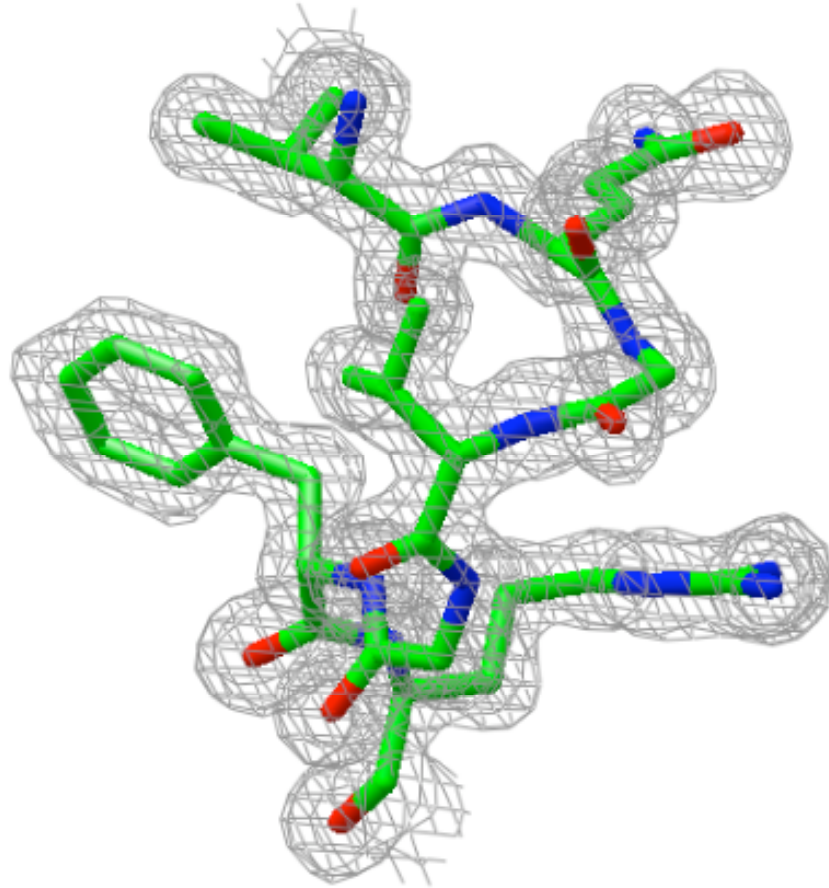
Presentation of an electron density isosurface (actually an iso-density surface) as a mesh of lines provides a transparent surface to which a model of a molecule can be compared and fit. This is called an isomesh.



An isomesh can be generated either by drawing planar contours in each of three independent directions or by computing the surface and approximating it by triangles (tessellation).

In the following examples, similar map data was used, in Xplor format, CCP4 map format and the evolving imgCIF/CBF format.

How CCP4MG Displays a Map



CCP4mg[5] display of 2fofc.map and 1w2i.pdb residues 14-20 and 38 from Chain A

CCP4MG Script To Render a Map

```
DT().filemenu.define_gui_openpdbfile(readpdb='1',widget = 'readpdb')
DT().filemenu.openpdbfile ( pdbin ='1w2i.pdb', ...)
DT().filemenu.openmtzfile(readmap='1',widget = 'readmap')
DT().filemenu.openmtzfile ( ccp4mapfile ='2fofc.map', ...)
disp('2fofc','2fofcMapDisp1').set_style('1.5')
disp('1w2i','1w2iMolDisp1').set_selection(_cid='1',widget = '_cid')

disp('1w2i','1w2iMolDisp1').set_selection( cid ='//A/14-
20,38 ', exit ='ok' )

disp('2fofc','2fofcMapDisp1').set_colour(colour='grey',wi
dget = 'colour')

disp('1w2i','1w2iMolDisp1').set_style(style_mode='CYLINDERS',widget =
'style_mode')
disp('2fofc','2fofcMapDisp1').set_selection(clip_atoms='1w2iMolDisp1',widg
et = 'clip_atoms')
```

```
disp('2fofc','2fofcMapDisp1').set_selection(clip_atoms='OFF',widget =  
'clip_atoms')
```

```
disp('2fofc','2fofcMapDisp1').centre_on(centre_on='1',widget = 'centre_on')
```

```
disp('2fofc','2fofcMapDisp1').set_selection(clip_atoms='point',widget =  
'clip_atoms')
```

```
disp('2fofc','2fofcMapDisp1').set_params(surface_style=  
chickenwire',widget = 'surface_style')
```

```
disp('2fofc','2fofcMapDisp1').set_style('1.0')
```

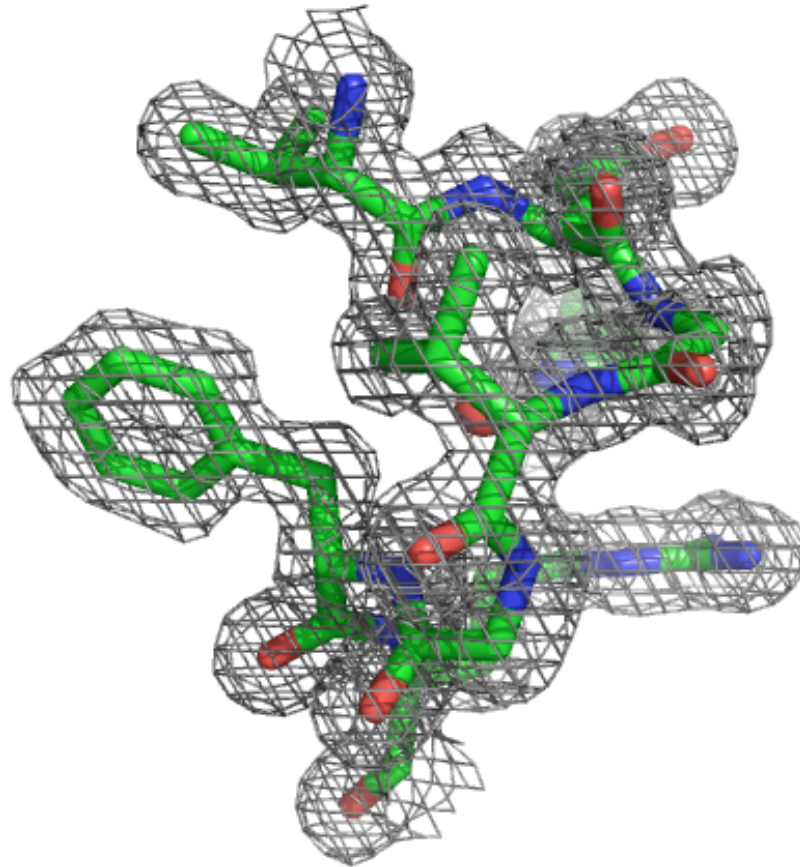
```
disp('2fofc','2fofcMapDisp1').set_selection(atom_clip_radius='other',widget  
= 'atom_clip_radius')
```

```
disp('2fofc','2fofcMapDisp1').set_selection( atom_clip_radius = '1.6', exit  
='ok' )
```

```
disp('Crystals','crystal').set_selection(source='1w2i',widget = 'source')
```

```
disp('2fofc','2fofcMapDisp1').set_selection(clip_atoms='1w2iMolDisp1',widg  
et = 'clip_atoms')
```


How PyMOL Displays a Map



PyMOL display of 1w2i.pdb and 2fofc.map.xplor[8], residues 14-20 and 38 from Chain A

PyMOL Script to Render a Map

```
CmdLoad: "C:/Program Files/DeLano
```

```
...
```

```
select active, (resi 14-20,38) and chain A
```

```
...
```

```
show sphere, active_water
```

```
alter active_water, vdw=0.5
```

```
rebuild
```

```
isomesh mesh1, 2fofc.map, 1.0, (resi 14-20,38 and chain  
A), carve=1.6
```

```
isomesh mesh1, 2fofc.map, 1.0, active, carve=1.6
```

```
color grey, mesh1
```

```
bg_color white
```

```
...
```

Proposed RasMol Handling of Maps

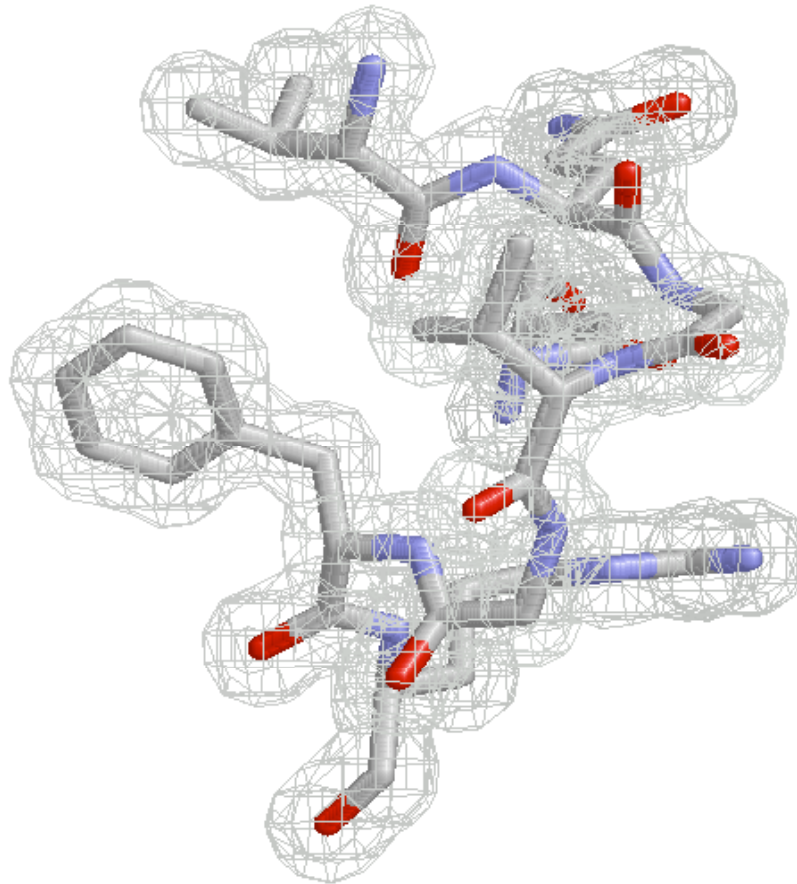
(Work in Progress, Comments appreciated)

load map <file path> or map load <file path>	}	Load a CBF or CCP4 map
map level <number> {MEAN} map spacing <number>	}	Set contour parameters
map generate map spread <number>	}	Generate map from atoms
map show or show map	}	Display map parameters

Objective: Simpler for users to understand, set defaults so that for most users “load map <file path>” loads and displays a reasonable map. SBEVSL will translate to other script formats

How RasMol Will Display a Map

(Work in Progress, Comments appreciated)



RasMol display of generated map and 1w2i.pdb, residues 14-20 and 38 from Chain A

SBEVSL

“Structural biologists and molecular scientists in many other disciplines need to communicate effectively about biological macromolecules. The number and complexity of available structures are both increasingly dramatically. There are many free molecular visualization programs that facilitate macromolecular structure analysis and experimental design. Each program has distinct features and limitations, often leading researchers to utilize multiple programs to successfully investigate all qualities of a macromolecular structure. To alleviate this problem, we are creating a common ontology called the Structural Biology Extensible Visualization Scripting Language (SBEVSL) that will serve as a central resource for communicating scripts between different visualization programs...” [1]

Examples of the Detail of Proposed Commands

{set} map level <number> {MEAN} - To change contour level before or after load. <number> is the electron density in electrons per Å³. The optional “MEAN” modifier allows the level to be set relative to the mean.

{set} map spacing <number> - To change the spacing between contour levels before or after load.

{set} map {dots|wireframe|solid|transparent} –
To change the map display format

map restrict/select <selection> - (to control how much of the contour surface is displayed). Show only the electron density associated with a selected set of

atoms (or residues or chains or specific map numbers). This is the same command that selects the atoms themselves. Each portion of a surface is associated with whichever atom is closest to it. The clause “map=<number>” allows commands to be directed to particular maps. The clause “within” can be used to specify a distance within which to accept both map surface elements and atoms.

The idea is to allow commands similar to those used in current programs but, by use of sticky selections, to allow the commands to be simple and closer to what is done with menus and mice.

Map File Formats

RasMol will support imgCIF/CBF and CCP4 format

imgCIF – Crystallographic Binary Format – supports several compressions including J. P. Abrahams pack_c.c compression and Hammersley’s byte offset compression. Byte offset compression allows use of compressed maps in memory. Simple tag-value structure, order independent, allows multiple maps, masks and other images in one file

CCP4 – important community standard for maps.

In both cases, while “real” maps can be compressed, logarithmic maps as scaled integers will offer better compression.

CCP4 Relation to imgCIF/CBF

1-3	NC, NR, NS	# of Columns, Rows, Sections CBF: <code>_array_structure_list.dimension</code>
4	MODE	Data type 0 = envelope stored as signed bytes 2 = Image stored as Reals CBF: <code>_array_structure.encoding_type</code>
5-7	NCSTART, NRSTART, NSSTART	
8-10	NX, NY, NZ	Number of intervals along X, Y, Z CBF: <code>_array_structure_list.dimension</code>
11-16	a, b, c, alpha, beta, gamma	Cell Dimensions CBF: <code>cell.length_a</code>
17-19	MAPC, MAPR, MAPS	Which axis corresponds to Cols, Rows, Sections. (1,2,3 for X,Y,Z) CBF: <code>_array_structure_list.precedence</code>
...		

Indexing Byte Offset Maps in Memory

The choice of map format has an impact on software performance. Newer computers can use memory resident maps, but compression is often needed. However, care is needed to avoid constant re-decompression of the same data.

Hammersley's byte offset compression records the byte-by-byte deltas as bytes, 16-bit integers or 32-bit integers. It does not compress as much as J. P. Abrahams' CCP4 pack_c.c compression but is very fast, is always byte aligned and decompression of the value of any pixel depends only on knowing the value of the immediately prior pixel. The compressed map itself is typically 1/4 the size of the original map for 32 bit integers. An index of every 256th byte location and value will add only 25% to the compressed size, and will allow portions of the map to be decompressed without rereading the entire map.

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References

- [1] C. Westin, B. Hanson, H. J. Bernstein, I. Awuah Asiamah, D. Boycheva, G. Darakev, N. Darakev, J. Jemilawon, N. Jia, P. Kamburov, G. Todorov, P. A. Craig, S. Mottarella, "SBEVSL: Communicating scripts between molecular visualization programs," Abstract E003, ACA 2007, Salt Lake City, UT, July 2007
- [2] W. L. DeLano, "The PyMOL Molecular Graphics System.", DeLano Scientific LLC, San Carlos, CA, USA. <http://www.pymol.org>
- [3] R. Sayle and E. J. Milner-White. "RasMol: Biomolecular graphics for all", Trends in Biochemical Sciences (TIBS), September 1995, Vol. 20, No. 9, p. 374.
- [4] H. J. Bernstein, "Recent changes to RasMol, recombining the variants", Trends in Biochemical Sciences (TIBS), September 2000, Vol. 25, No. 9, pp. 453-455.
- [5] L. Potterton, S. McNicholas, E. Krissinel, J. Gruber, K. Cowtan, P. Emsley, G. N. Murshudov, S. Cohen, A. Perrakis and M. Noble, "Developments in the CCP4 molecular-graphics project", *Acta Cryst.* (2004). D60, pp. 2288-2294
- [6] A. Paehler (2004, November 11). About the PDBj Electron Density Map Viewer. Retrieved April 7, 2007, from <http://133.1.158.159/about.html>
- [7] ccp4mg display of toxd_sfall1.map [http://www-structmed.cimr.cam.ac.uk/phaser/tutorial/Phaser MR tute.html](http://www-structmed.cimr.cam.ac.uk/phaser/tutorial/Phaser_MR_tute.html)
- [8] PyMOL Viewer 2fofc.map.xplor with electron density displayed around the active site atoms at sigma level=1.0
- [9] A. Philippsen. DINO: Visualizing Structural Biology (2003) <http://www.dino3d.org>