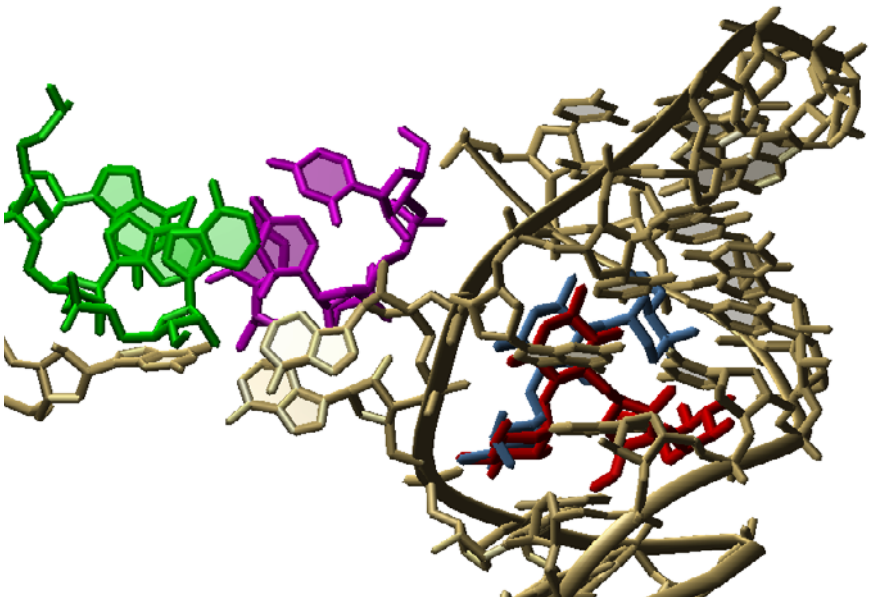
Supplementary information S1 (box)

A few years ago, modelling and visualizing a structure the size of a ribosomal subunit was in the domain of supercomputers and graphical workstations. Now, owing to the increased power of computer processors, it is possible to view these structures on relatively inexpensive PCs sold on the commercial market. Obtaining software to display and interpret the crystal structures is also straightforward, and there is an abundance of good, freely-available software packages that can be downloaded from the internet. As ribosomes are much larger than other structures normally studied, not all of the programs were designed to cope with this amount of data. A selection of free software that we found helpful for handling the ribosome structures are listed below:

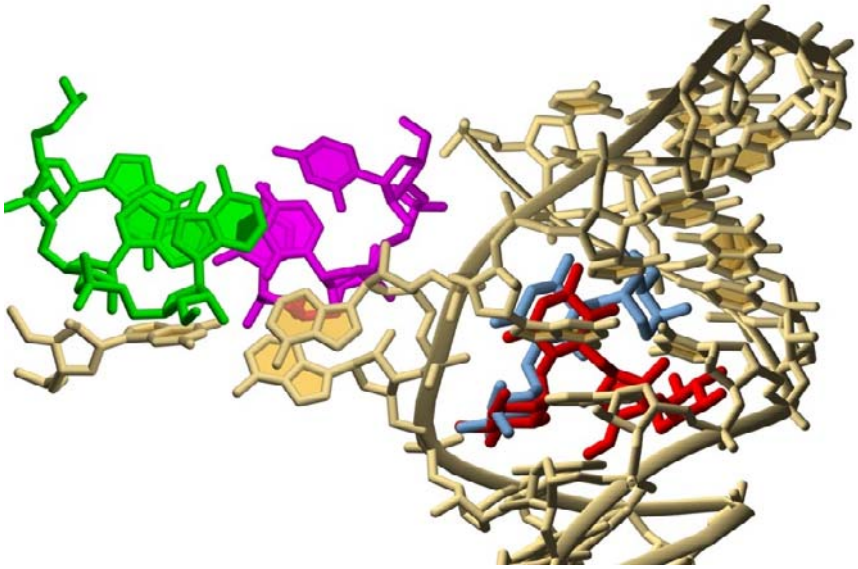
Program	**URL**
Chime	http://www.umass.edu/microbio/chime/
Chimera	http://www.cgl.ucsf.edu/chimera/
Cn3D	http://www.biosino.org/mirror/www.ncbi.nlm.nih.gov/Structure/cn3d/cn3d.html
Molmol	http://hugin.ethz.ch/wuthrich/software/molmol/
MolPov	http://www.chem.ufl.edu/~der/der_pov2.htm
MolScript	http://www.avatar.se/molscript/
PovRay	http://www.povray.org/
Pymol	http://pymol.sourceforge.net/
Rastop	http://www.geneinfinity.org/rastop/
Ribbons	http://sgce.cbse.uab.edu/ribbons/
SPDBV (DeepWiew)	http://www.expasy.org/spdbv/
VMD	http://www.ks.uiuc.edu/Research/vmd/

In addition to viewing individual structures, many of the software packages enable superposition of two or more data sets using atoms in common structural features as anchor points. The visualisation programs also offer different molecular graphics (for example, variations of ball-and-stick models or molecular surface representations) to enable one to focus on particular structural aspects. Initial confrontation with some of the graphics software will require a steep learning curve, although most programs are reasonably well explained. Some of the programs allow the user to export data to a generic 3D modelling program to enhance the appearance and to carry out further 3D work. A good example of this is the Pov-Ray program, which is freely available for download. Pov-Ray takes a data-file from the molecular visualisation programs and adds true light-sourced shadows, creating a sense of depth and enabling creation of high-resolution pictures suitable for printing:

Screenshot from MolMol:



The same screenshot rendered in Pov-ray:



This picture was made using a structure of the 30S ribosomal subunit in complex with cognate tRNA and mRNA fragments, and binding the aminoglycoside antibiotic, paromomycin (acc. number 1IBL). Geneticin was docked into this complex using the crystal structure of a small artificial 16S fragment with the antibiotic bound (acc. number: 1MWL). The two structures were aligned using the backbone atoms of the RNA.