Making pretty pictures
So how does one go about solving a crystal structure?

<table>
<thead>
<tr>
<th>Step</th>
<th>Details</th>
<th>Responsible Party</th>
</tr>
</thead>
<tbody>
<tr>
<td>formulate question</td>
<td>very hard!</td>
<td>Boss</td>
</tr>
<tr>
<td>make sample</td>
<td>cloning, expression, purification</td>
<td>you</td>
</tr>
<tr>
<td>make crystal</td>
<td>screening, optimisation</td>
<td>you</td>
</tr>
<tr>
<td>collect diffraction data</td>
<td>synchrotron, integration, scaling</td>
<td>Post-doc</td>
</tr>
<tr>
<td>solve phase problem</td>
<td>MR, SIRAS, MIRAS, SAD, MAD, hybrid</td>
<td>Post-doc/Randy/Phil</td>
</tr>
<tr>
<td>build model</td>
<td>manual or autotracing</td>
<td>Post-doc/you</td>
</tr>
<tr>
<td>refine model</td>
<td>agreement of model and data</td>
<td>Post-doc/Garib</td>
</tr>
<tr>
<td>interpret model</td>
<td>very hard! back to top?</td>
<td>Boss</td>
</tr>
<tr>
<td>write paper</td>
<td>read lots of lit, come up with model</td>
<td>Boss</td>
</tr>
<tr>
<td>make figures</td>
<td>.....</td>
<td>you</td>
</tr>
</tbody>
</table>

After all this work, you only have one chance to communicate your results. So you better make the most of it.
Published Figure!
COLOURS

RGB

CMYK

http://www.scottefranson.com/3-books/publishing/tutorials/tutorial-color.html
COLOURS

**ADDITIVE**

RGB
red/green/blue

**SUBTRACTIVE**

CMYK
cyan/magenta/yellow/black

HSB
hue/saturation/brightness
Journal 1
“All colour artwork must be submitted in CMYK colour mode. When converting files from RGB, please consider that the final figures will be printed on coated paper, using Euroscale process inks. If you are not familiar with these specifications, or are not sure how to apply them within your software package, please consult a local graphics expert.”

Journal 2
“Color figures must be prepared in RGB color mode, not CMYK. The journal uses the RGB format to optimize color performance for online publication.”
In Pymol: Display > Colour Space > CMYK
or: cmd.space (‘cmyk’)
In Photoshop: Image > Mode > CMYK
In Illustrator: File > Document mode > CMYK
In Powerpoint: select object > fill > colour sliders > RGB/CMYK/HSB
Colour blind people cannot discriminate between red and green.
Colour Blindness

One in twelve Caucasian (8%), one in 20 Asian (5%), and one in 25 African (4%) males are so-called "red-green" colorblind.

From: http://jfly.iam.u-tokyo.ac.jp/color/
## Set of colors that is unambiguous both to colorblinds and non-colorblinds

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Black</td>
<td>-</td>
<td>(0,0,0,100)</td>
<td>(0,0,0)</td>
<td>(0,0,0)</td>
</tr>
<tr>
<td>2</td>
<td>Orange</td>
<td>41</td>
<td>(0,50,100,0)</td>
<td>(230,159,0)</td>
<td>(90,60,0)</td>
</tr>
<tr>
<td>3</td>
<td>Sky Blue</td>
<td>202</td>
<td>(80,0,0,0)</td>
<td>(86,180,233)</td>
<td>(35,70,90)</td>
</tr>
<tr>
<td>4</td>
<td>bluish Green</td>
<td>164</td>
<td>(97,0,75,0)</td>
<td>(0,158,115)</td>
<td>(0,60,50)</td>
</tr>
<tr>
<td>5</td>
<td>Yellow</td>
<td>56</td>
<td>(10,5,90,0)</td>
<td>(240,228,66)</td>
<td>(95,90,25)</td>
</tr>
<tr>
<td>6</td>
<td>Blue</td>
<td>202</td>
<td>(100,50,0,0)</td>
<td>(0,114,178)</td>
<td>(0,45,70)</td>
</tr>
<tr>
<td>7</td>
<td>Vermillion</td>
<td>27</td>
<td>(0,80,100,0)</td>
<td>(213,94,0)</td>
<td>(80,40,0)</td>
</tr>
<tr>
<td>8</td>
<td>reddish Purple</td>
<td>326</td>
<td>(10,70,0,0)</td>
<td>(204,121,167)</td>
<td>(80,60,70)</td>
</tr>
</tbody>
</table>

COLOURS – and lack thereof
Resolution and dpi (dots per inch)
On screen: 200 dpi
On paper: 300 dpi
But for line figures: 1000 dpi

(Guide to authors: “Non-vector graphics should be preserved at high resolution: 300 dpi minimum at final size for greyscale or colour halftone images, and 1,000 dpi minimum for bitmap (b/w) artwork.”

interaction motif is located at each end of this C-terminal segment. The first motif (residues 920-924) (Dohrmann and McHenry, 2003) is located just nine residues after the end of the crystal structure, while the second is located near the very C terminus of the full-length protein (residues 1154-1159) (Lopez de Saro et al., 2003). In addition, an OB domain (residues 994-1073) is located in the middle of the C-terminal segment, with strongest sequence similarity to the OB domain of the tRNA synthetase anticodon binding domain according to the PFAM database (Bateman et al., 2004). OB domains in other proteins are involved in protein-nucleic acid and protein-protein interaction (Theobald et al., 2003).

To further investigate the roles of the two β-clamp binding motifs and the OB domain we have generated a series of C-terminal deletion constructs of Pol III that were tested in a replication assay (Figure 6A). In this assay, singly primed M13 ssDNA coated with single-stranded DNA binding protein (SSB) is used to monitor DNA synthesis by the core subcomplex of the Pol III holoenzyme containing Pol III (the α subunit of the Pol III holoenzyme), the 3'-5' exonuclease ε, and the θ subunit (a small domain of uncertain function). In the absence of the β clamp and clamp loader, Pol III core shows distributive rather than processive synthesis and is incapable of replicating the M13 DNA (Figure 6B and Figure S4). In the presence of the clamp and clamp loader, Pol III core shows highly processive DNA synthesis, replicating the 7.2 kb M13 DNA rapidly. When the extreme C-terminal β clamp binding motif is deleted (Pol III1211, truncated at residue 1121), processive synthesis is still observed, albeit with less efficiency than for the wild-type Pol III core. When the OB domain
Figure 5. Model for DNA Binding in Pol III
(A) Surface representation of Pol III, with DNA indicated, is shown. The view is similar to that in Figure 1A. (B) Close up of the DNA-exit path, looking down the DNA axis, is shown. Several positively charged residues (colored in yellow) form an arch that contacts the backbone of the DNA. Active site residues are colored in black. (C) Close up view of a surface representation of the active site with conserved residues are represented in green. The viewpoint is along the arrow in panel (A). (D) Same view of the active site is shown with the catalytic triad in black sticks and residues that may be involved in nucleotide binding in yellow.

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Accession Numbers

The structures described in our paper have been deposited in the Protein Data Bank under ID codes 2HQA and 2HNH.
Vector and pixel based drawing

**Vector**
- Illustrator
- Powerpoint
- Canvas
- Coreldraw
- InkScape

**Pixel (bitmap)**
- Photoshop
- Gimp
- iPhoto
- ...

(vector)
(tiff)
(png)
(jpeg)
Representation & labeling

- PHP domain (cyan)
- Thumb domain (green)
- Palm domain (magenta)
- Fingers domain (red/brown)
For side chains create a separate object
Don’t show mainchain
Don’t do fancy intros.....
No shadows
Mismatch repair
Vitamin B12 transport
Double strand break repair
Mismatches repair

BtuCD
RAD50
MutS

Representation & labeling
Getting the message across

How much detail?
Getting the message across
Getting the message across

Inma Dorado
Little bit about movies
Little bit about movies

E. coli Pol III: Lamers 2006, Cell
Taq Pol III: Bailey 2006, Cell
Little bit about movies

Make movies start automatically
(so it doesn’t require that you click on the movie to start)
Movies > timing > start on click or start with previous

Create pauses during talk so you don’t have to rush through the movie
(i.e. create separate movies)

Morphing is a GREAT way to show differences between structures
(Use the Yale morph server or Chimera)
It doesn’t have to be fancy to be pretty...