Making pretty pictures

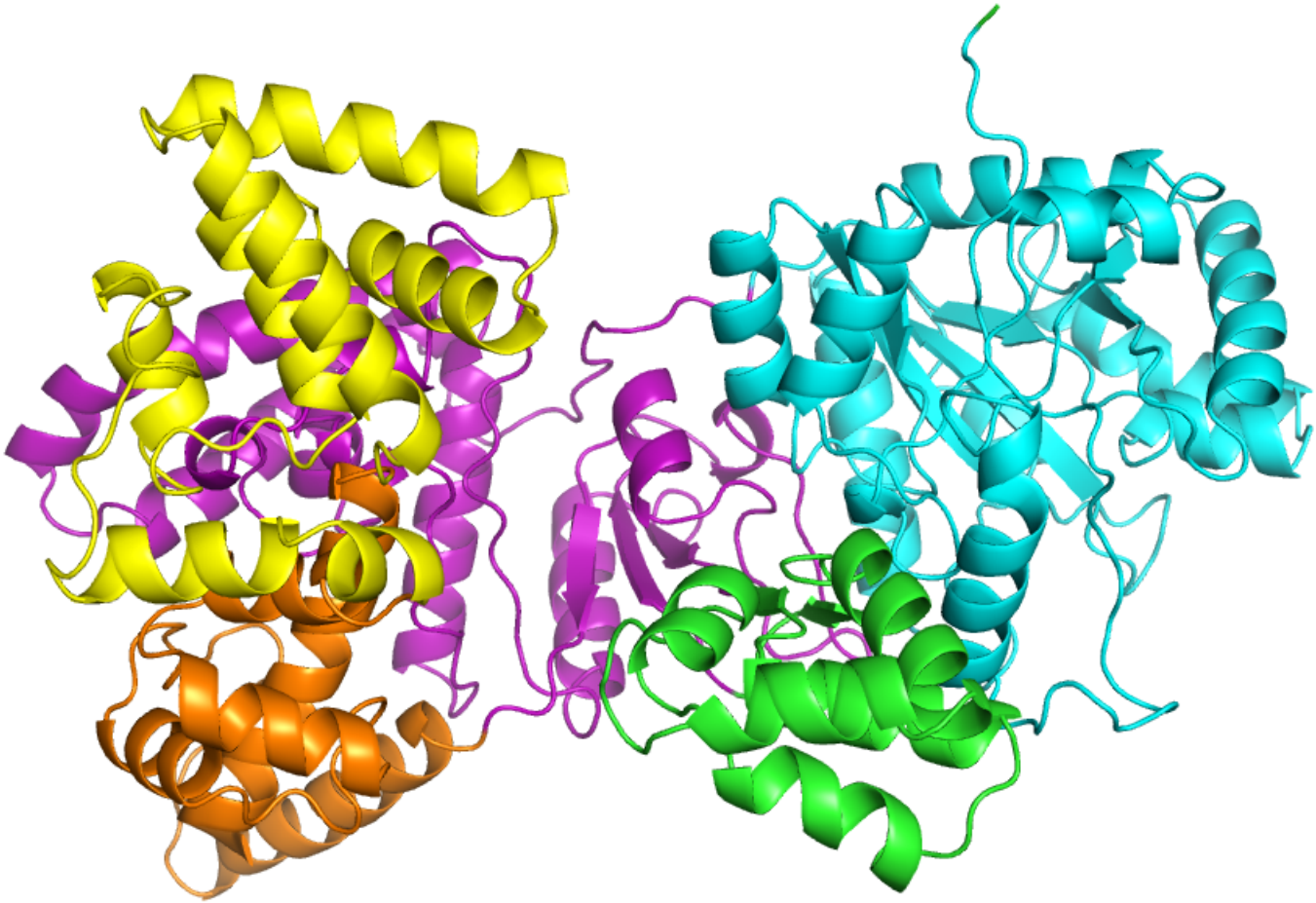
MAKING FIGURES

So how does one go about solving a crystal structure?

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

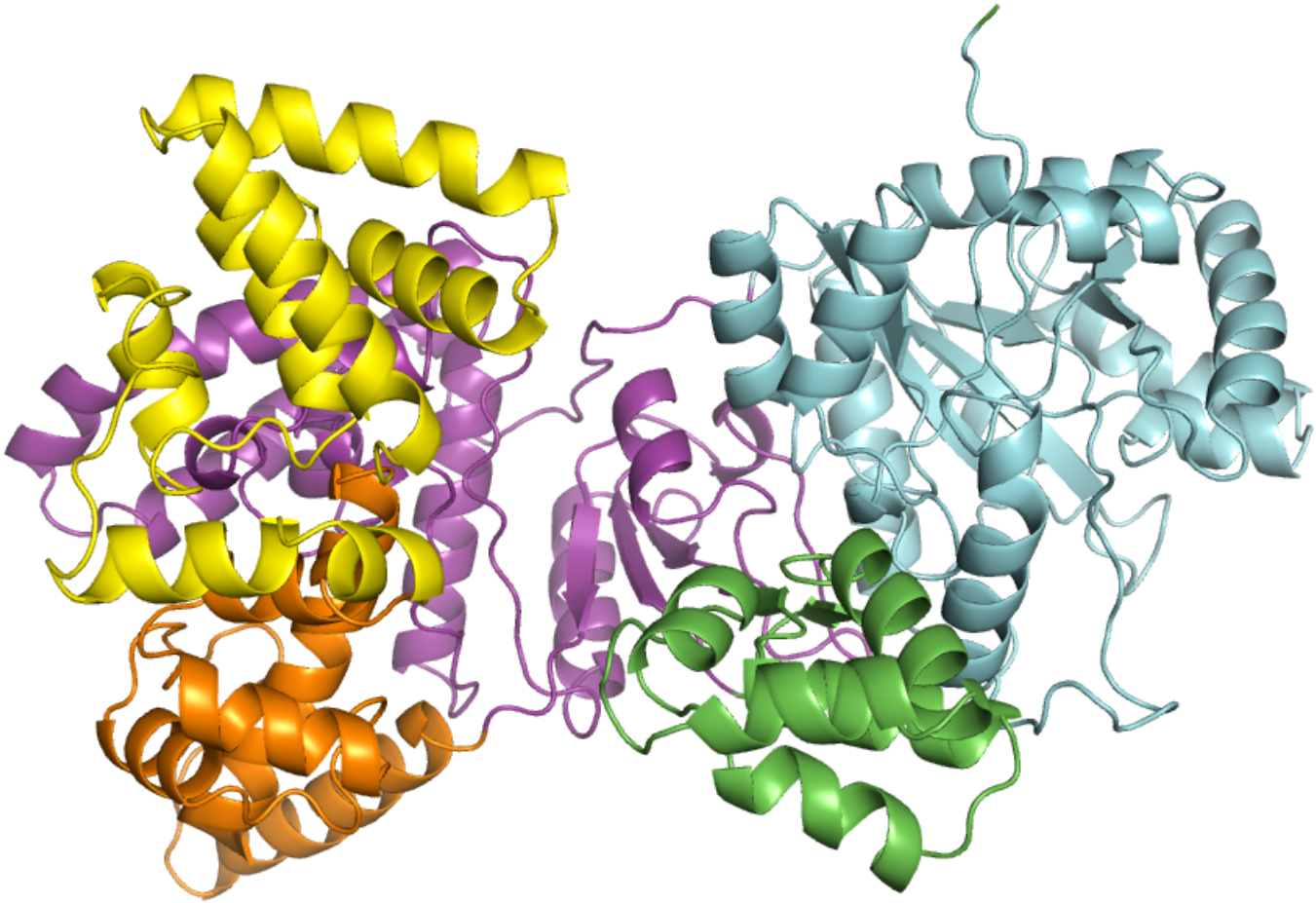
After all this work, you only have one chance to communicate your results. So you better make the most of it.

COLOURS



Original Figure

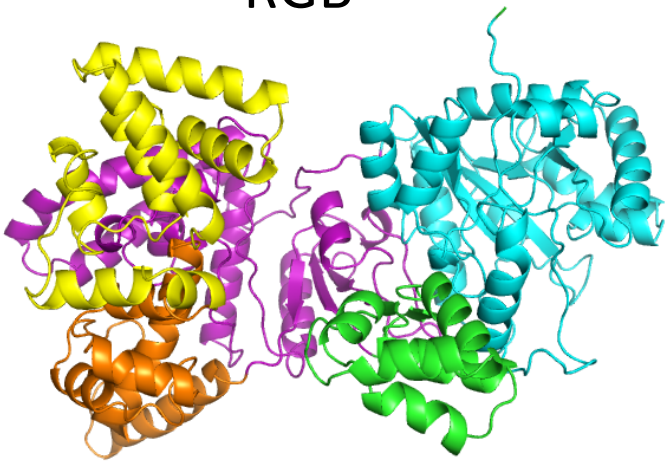
COLOURS



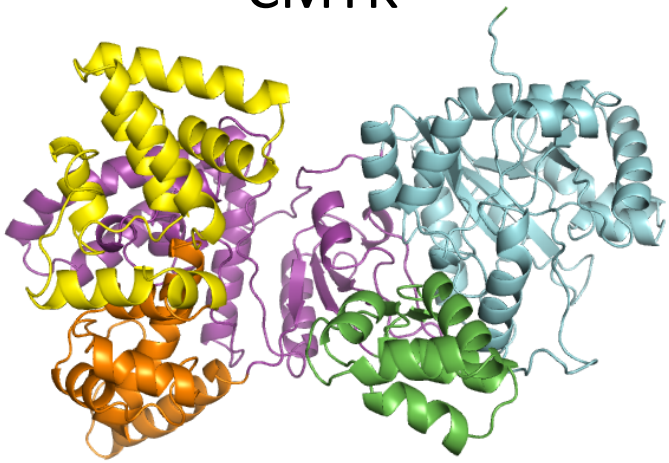
Published Figure!

COLOURS

RGB



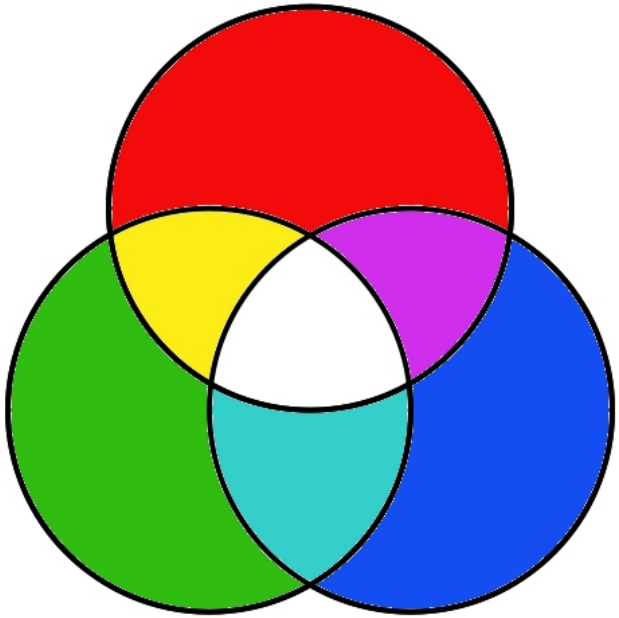
CMYK



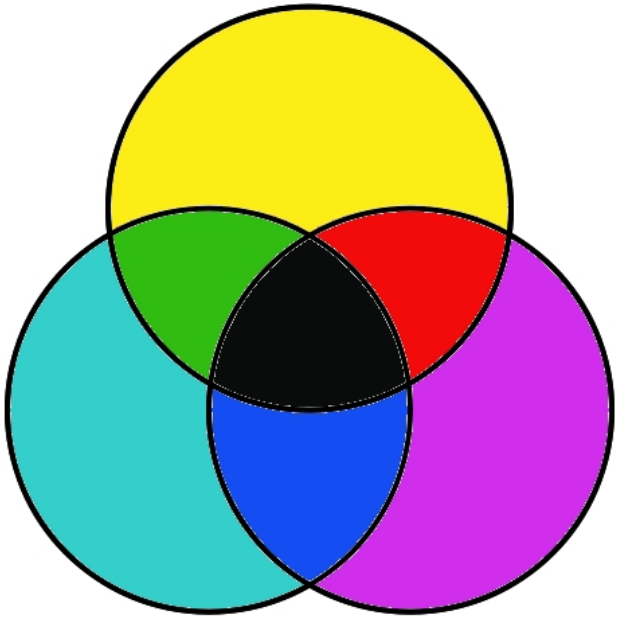
http://www.scottefranson.com/3-books/publishing/tutorials/tutorial-color.html

COLOURS

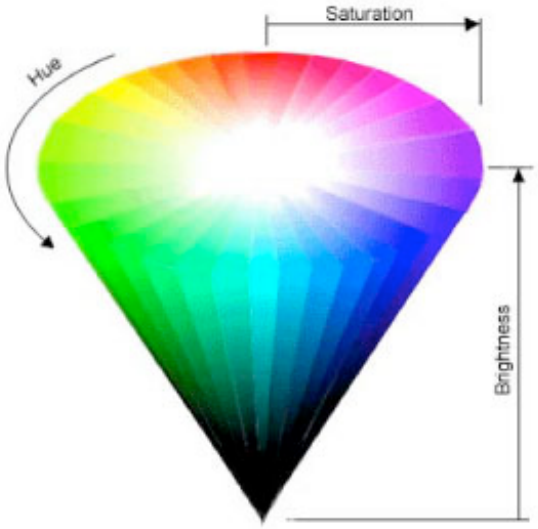
ADDITIVE



SUBTRACTIVE



RGB
red/green/blue



CMYK
cyan/magenta/yellow/black

HSB
hue/saturation/brightness

COLOURS

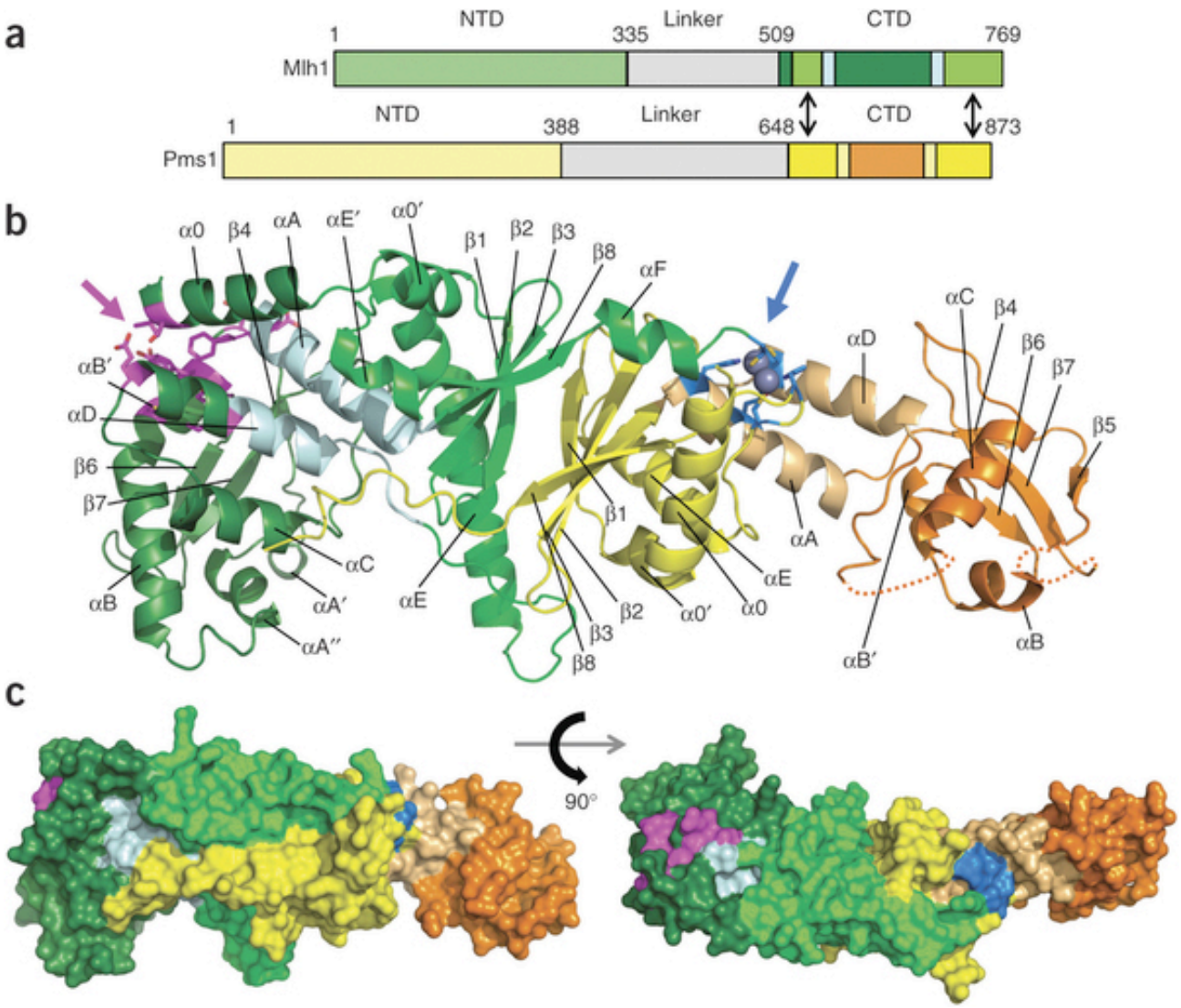
Journal 1

"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."

COLOURS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CTD
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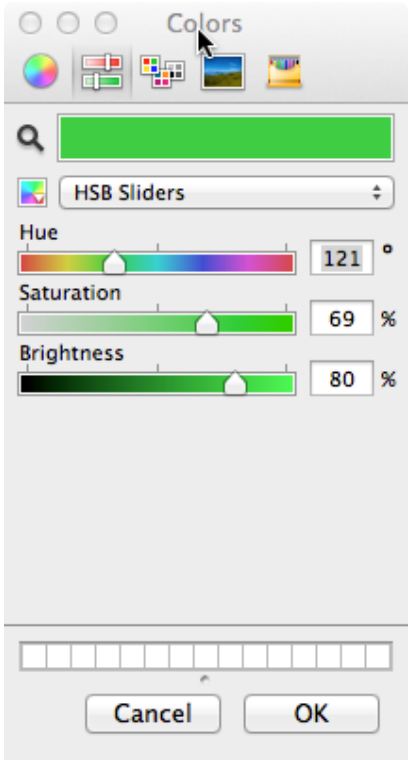
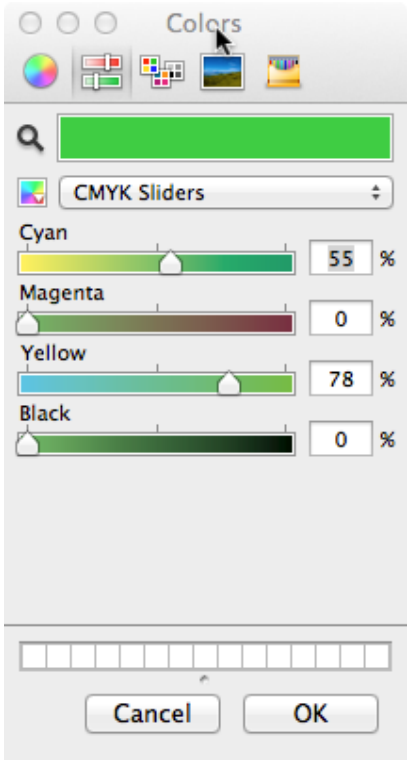
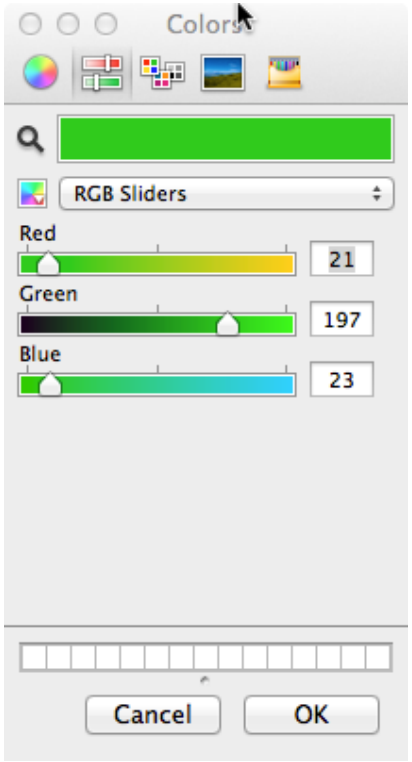
Pms1
b
α0
β4
αA
αE′
α0′
β1
β2
β3
β8
αF
αB′
αD
β6
β7
αC
αB
αA′
αA″
αE
β1
β2
β3
β8
α0′
α0
αE
αA
αD
αC
β4
β6
β7
β5
αB′
αB
c
90°

COLOURS

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

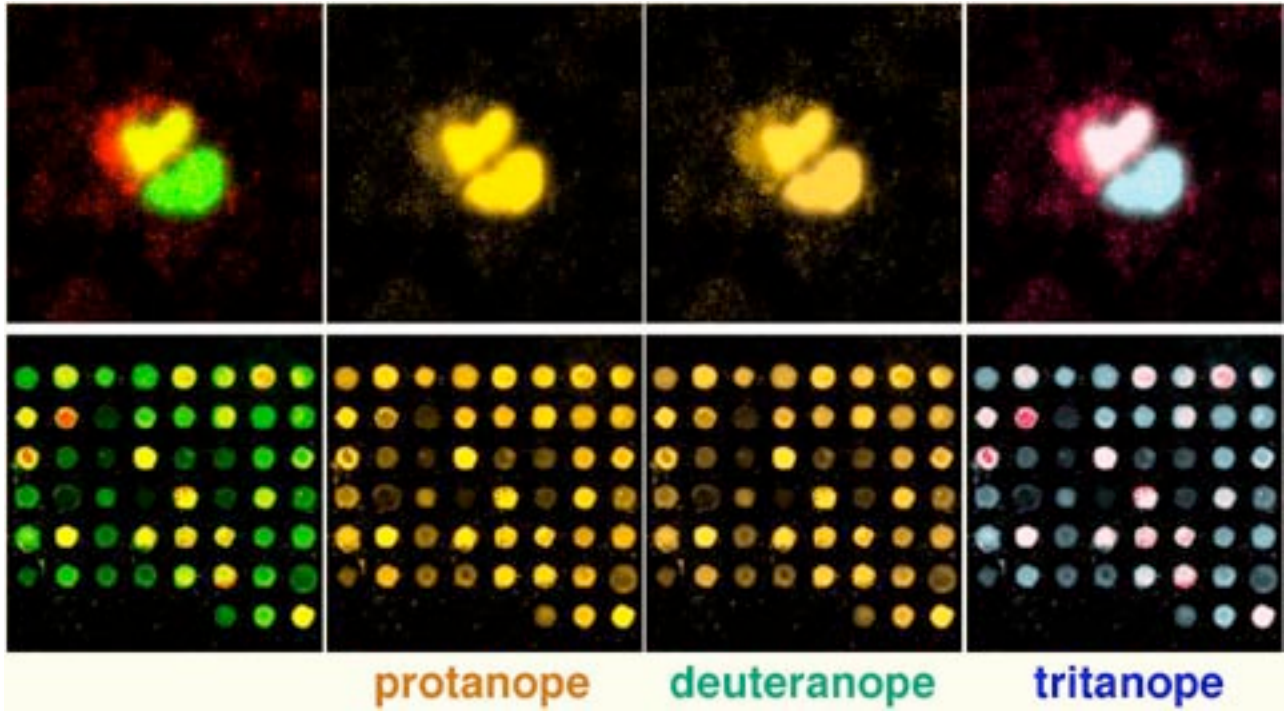






COLOURS – and lack thereof

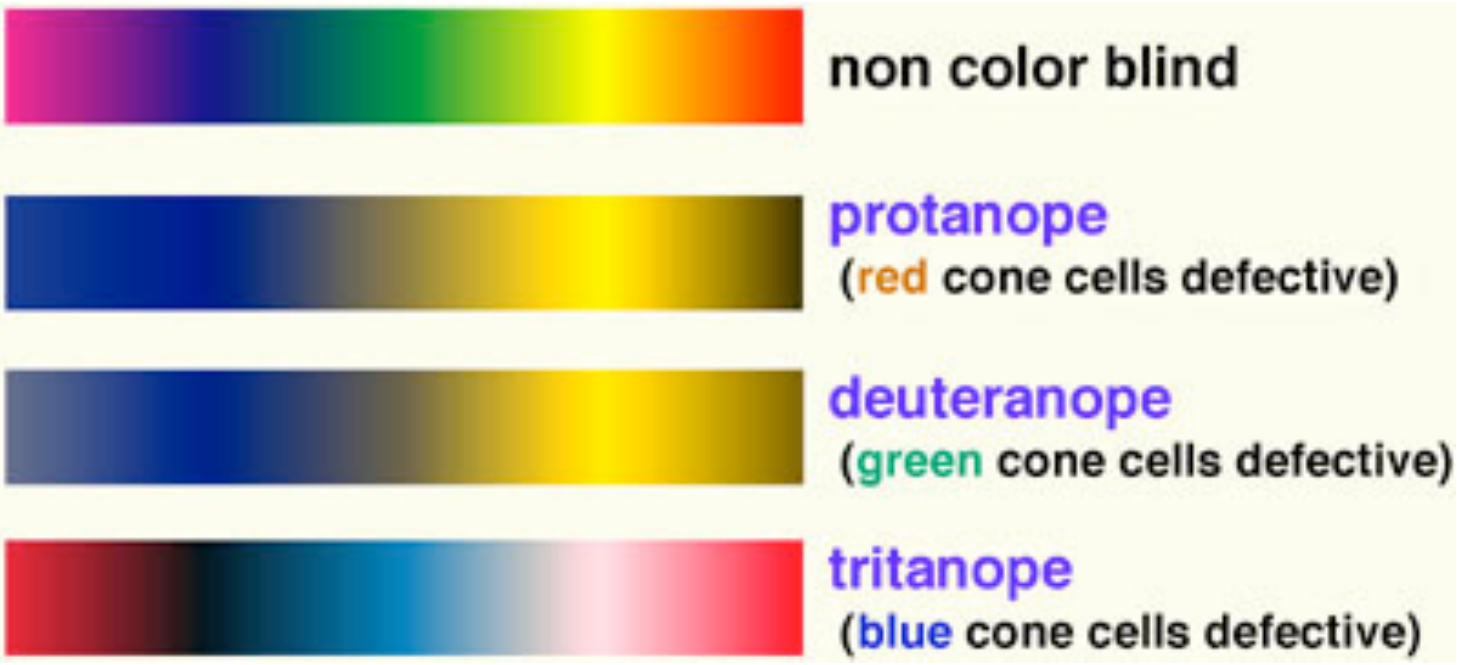
Colour blind people cannot discriminate between red and green



COLOURS – and lack thereof

Colour Blindness

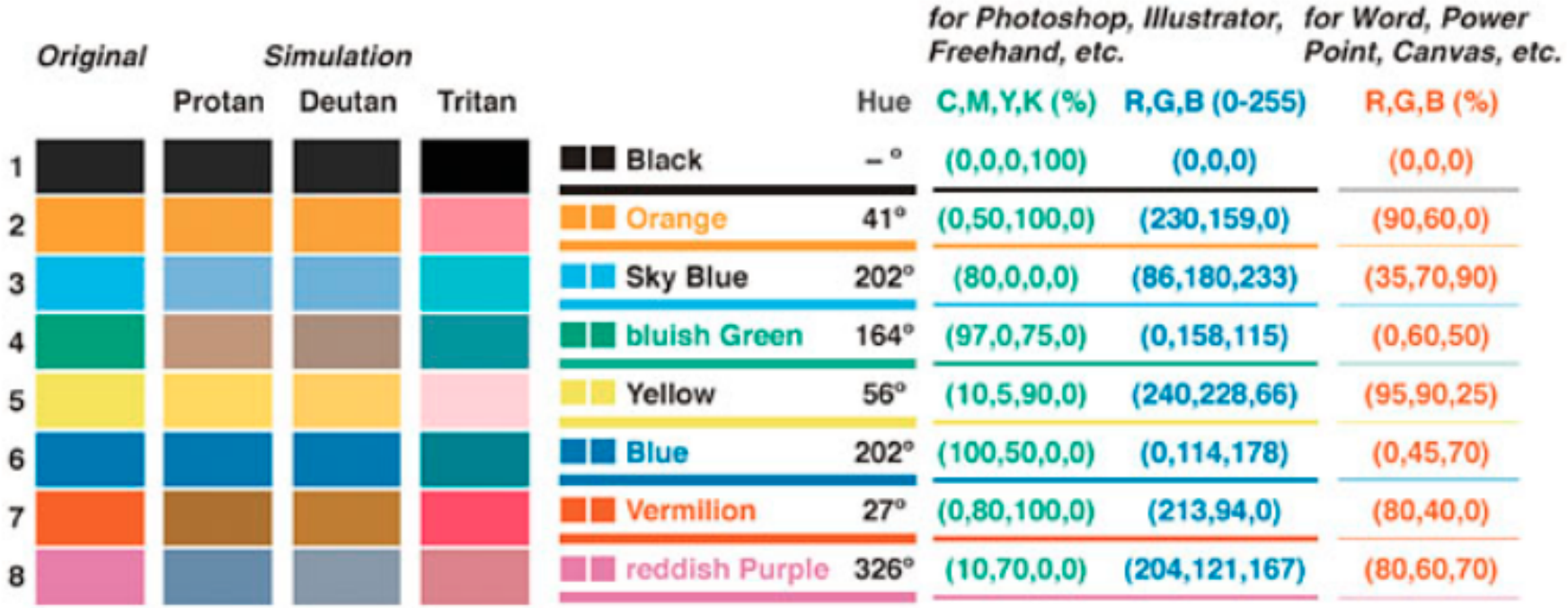
One in twelve Caucasian (8%), one in 20 Asian (5%), and one in 25 African (4%) males are so-called "red-green" colorblind.



From: http://jfly.iam.u-tokyo.ac.jp/color/

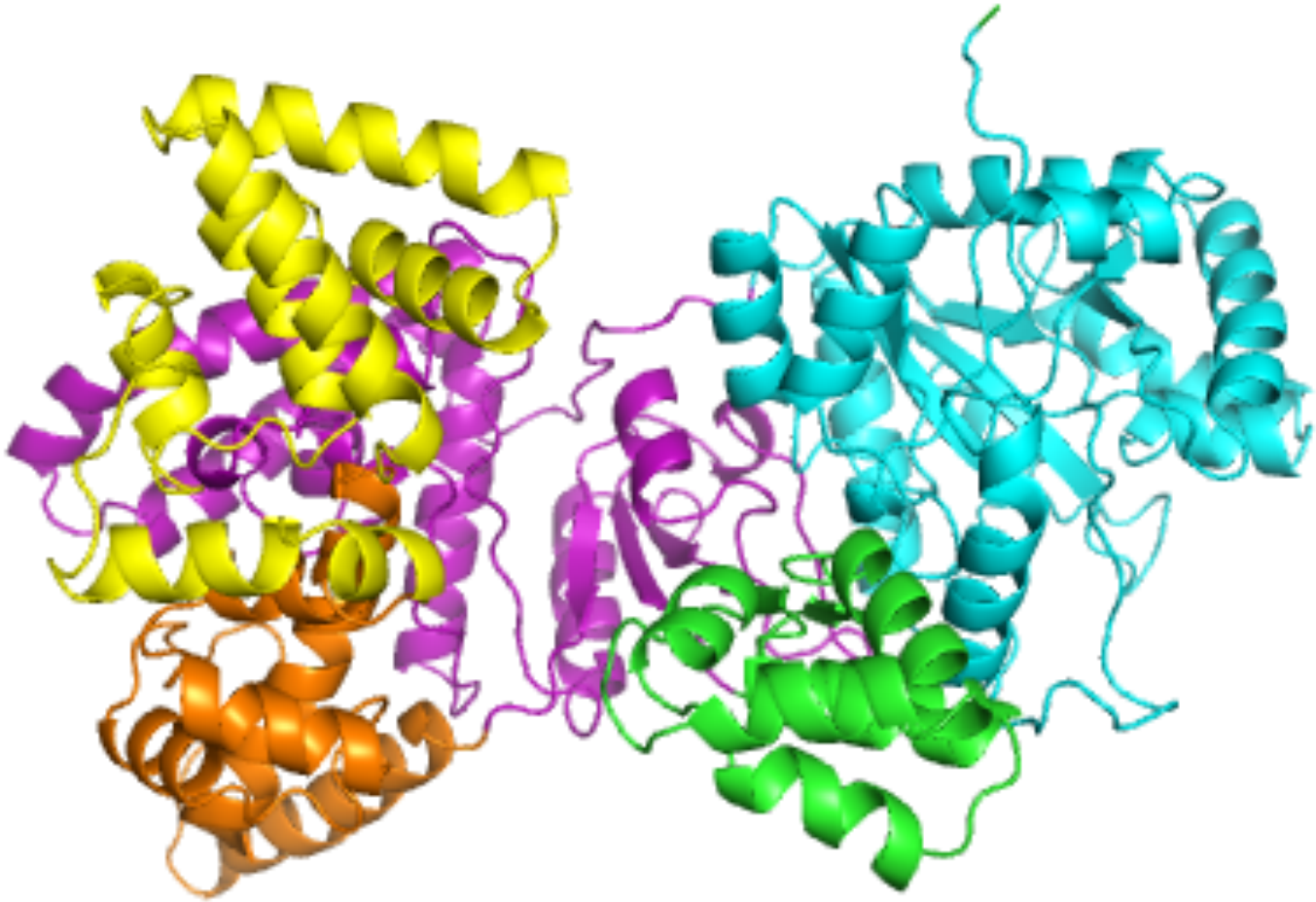
COLOURS – and lack thereof

Set of colors that is unambiguous both to colorblinds and non-colorblinds



	Original	Simulation: Protan	Simulation: Deutan	Simulation: Tritan		Hue	for Photoshop, Illustrator, Freehand, etc.: C,M,Y,K (%)	for Photoshop, Illustrator, Freehand, etc.: R,G,B (0-255)	for Word, Power Point, Canvas, etc.: R,G,B (%)
1					Black	– °	(0,0,0,100)	(0,0,0)	(0,0,0)
2					Orange	41°	(0,50,100,0)	(230,159,0)	(90,60,0)
3					Sky Blue	202°	(80,0,0,0)	(86,180,233)	(35,70,90)
4					bluish Green	164°	(97,0,75,0)	(0,158,115)	(0,60,50)
5					Yellow	56°	(10,5,90,0)	(240,228,66)	(95,90,25)
6					Blue	202°	(100,50,0,0)	(0,114,178)	(0,45,70)
7					Vermilion	27°	(0,80,100,0)	(213,94,0)	(80,40,0)
8					reddish Purple	326°	(10,70,0,0)	(204,121,167)	(80,60,70)

PIXELS AND MORE



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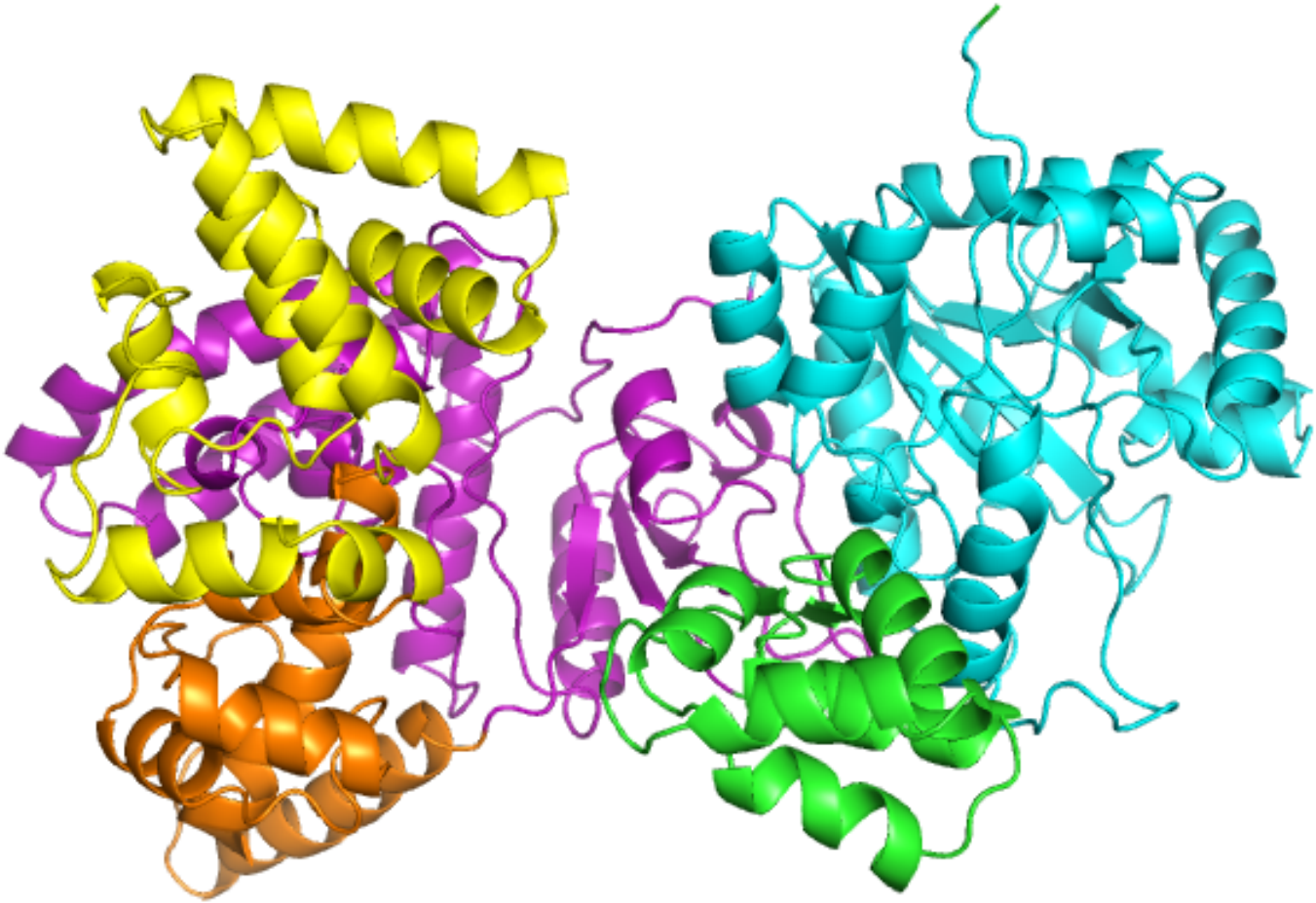
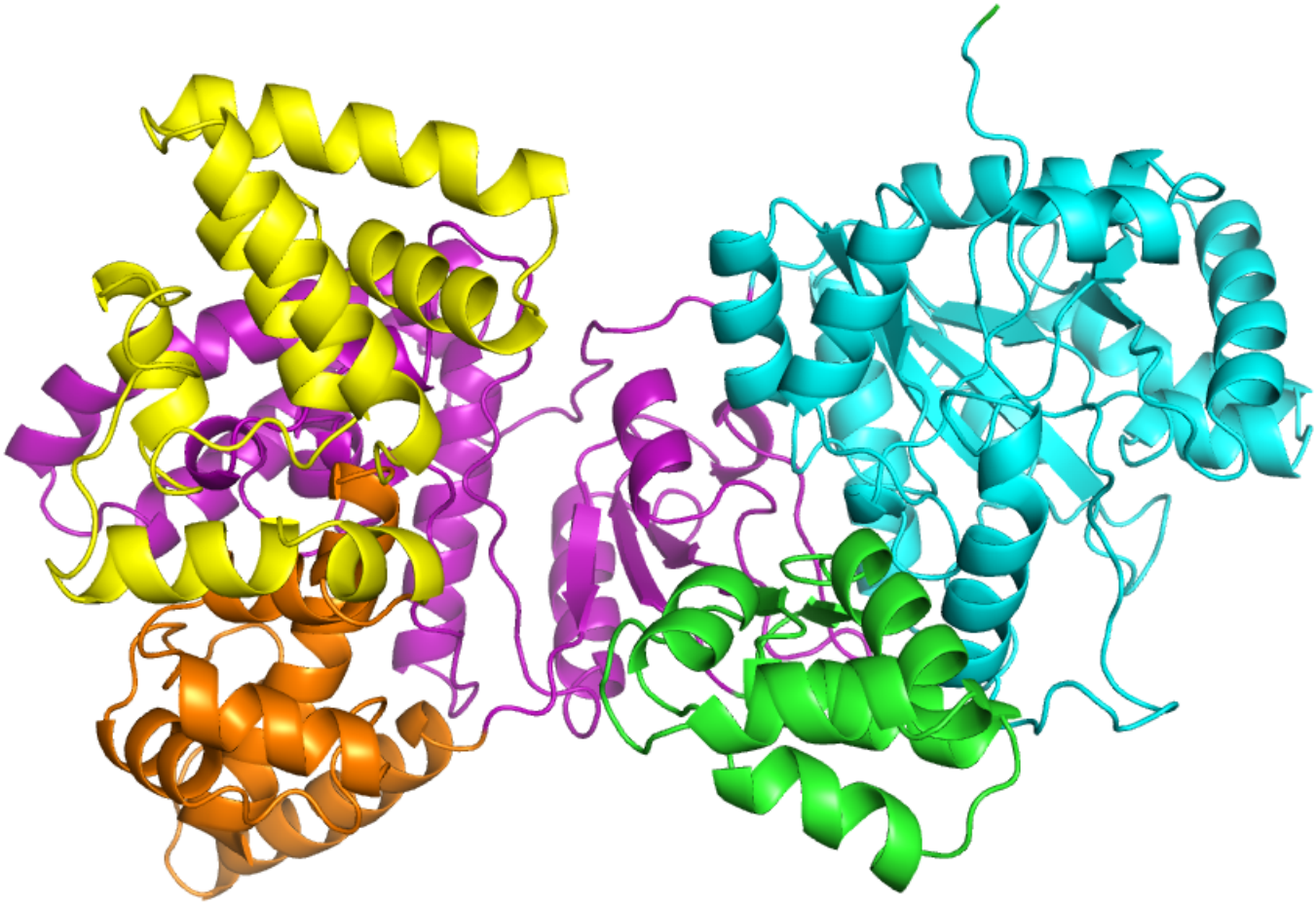
PIXELS AND MORE



600x600
(209KB)

PIXELS AND MORE



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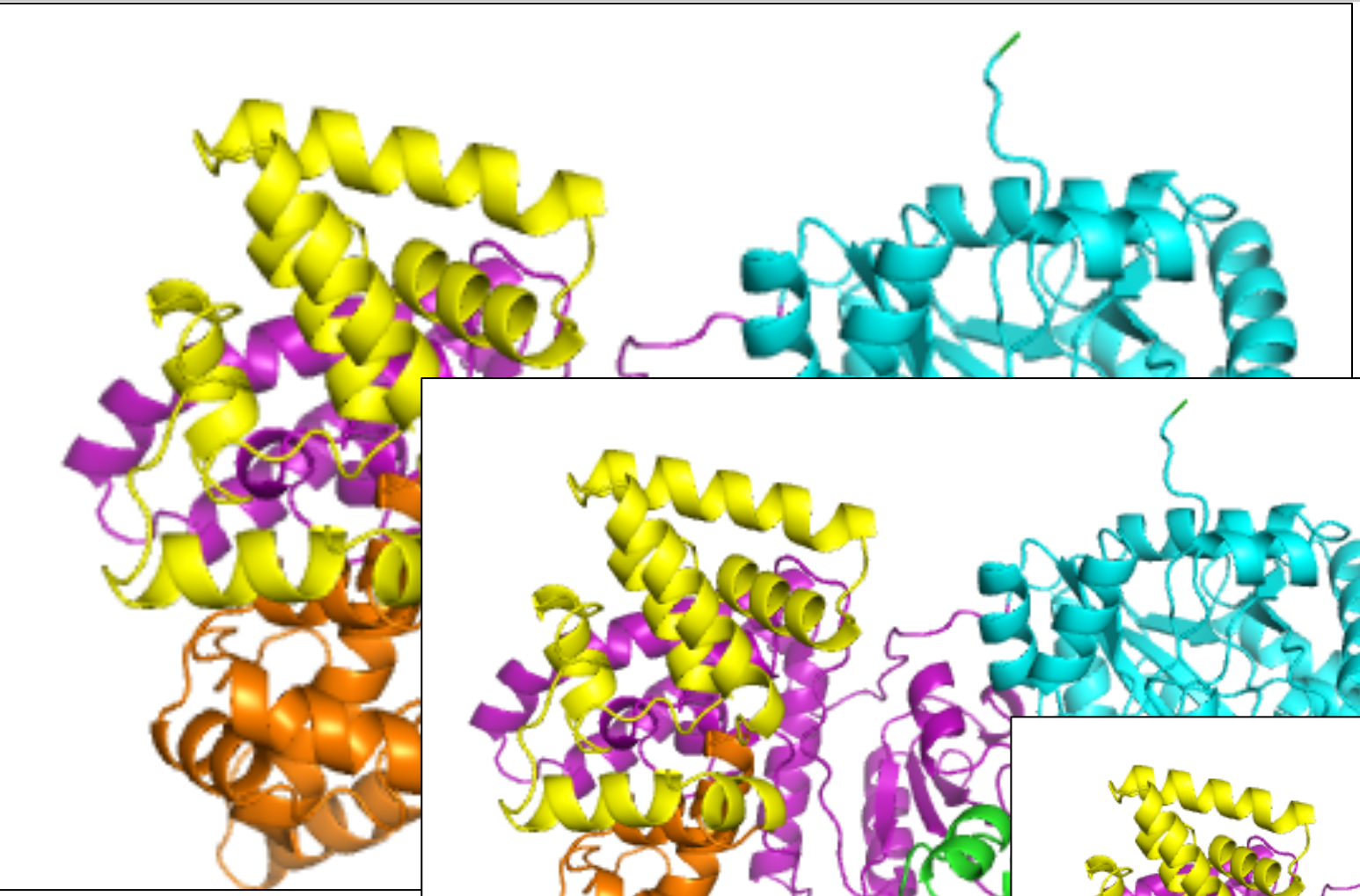
PIXELS AND MORE



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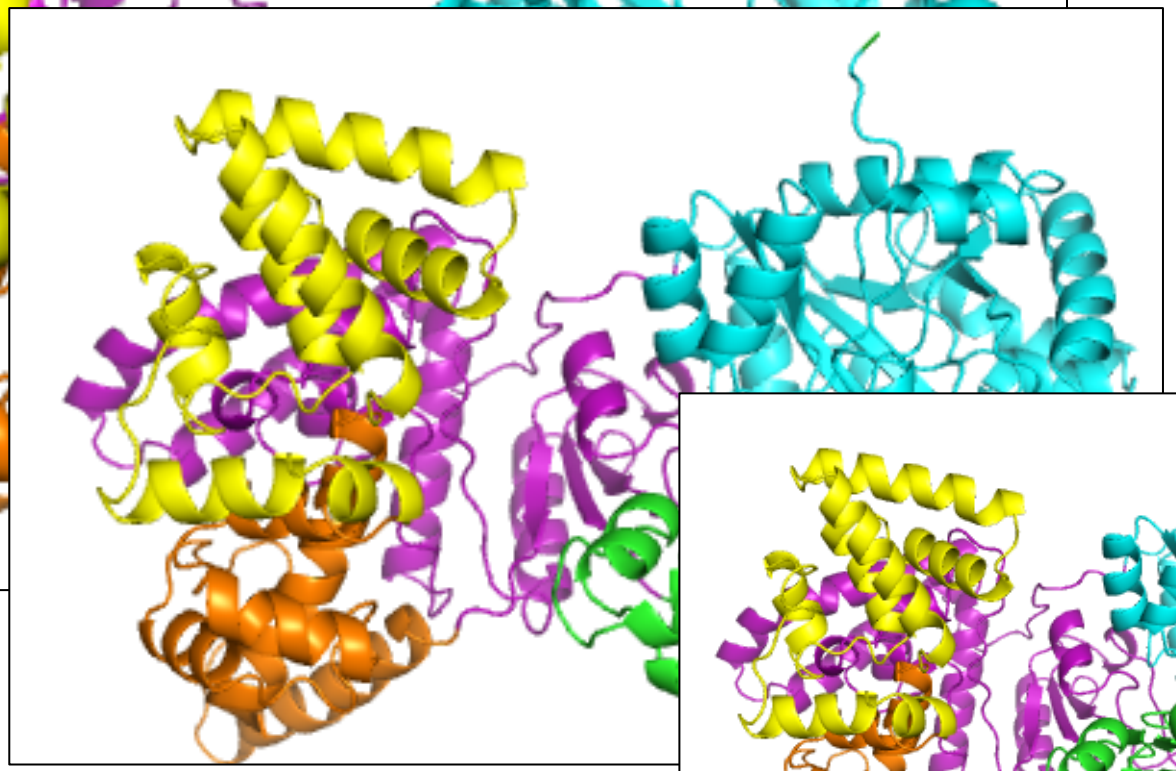

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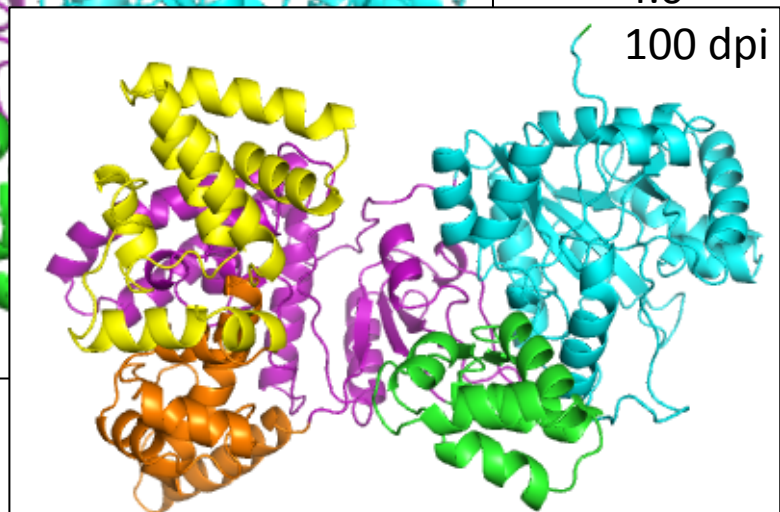


4.0”
100 dpi

Resolution and dpi (dots per inch)

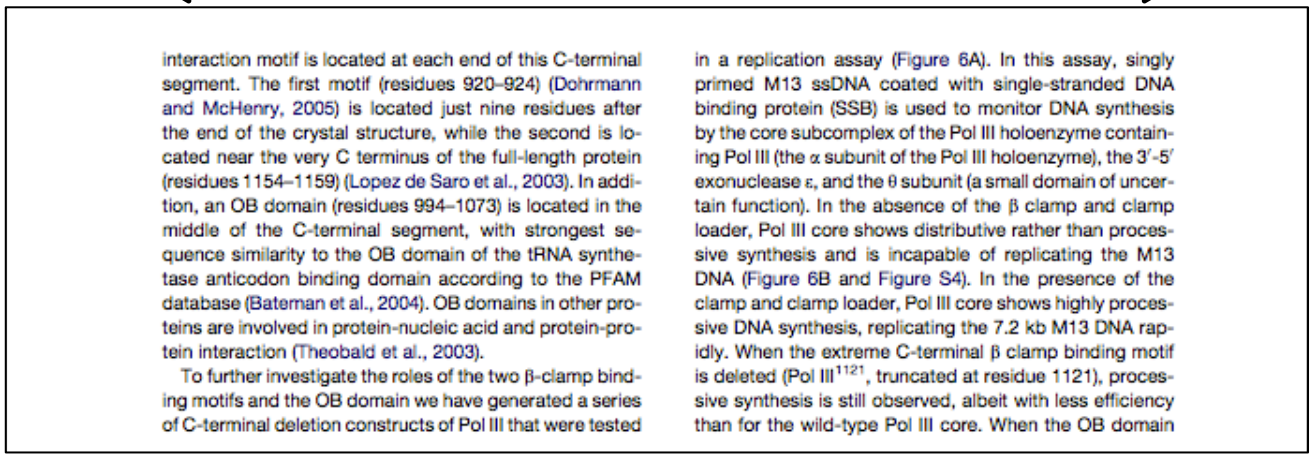
PIXELS AND MORE

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.”

3.5 inch: 1050 pixels

7.2 inch: 2160 pixels



interaction motif is located at each end of this C-terminal segment. The first motif (residues 920–924) (Dohrmann and McHenry, 2005) 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 III^{1121}, 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

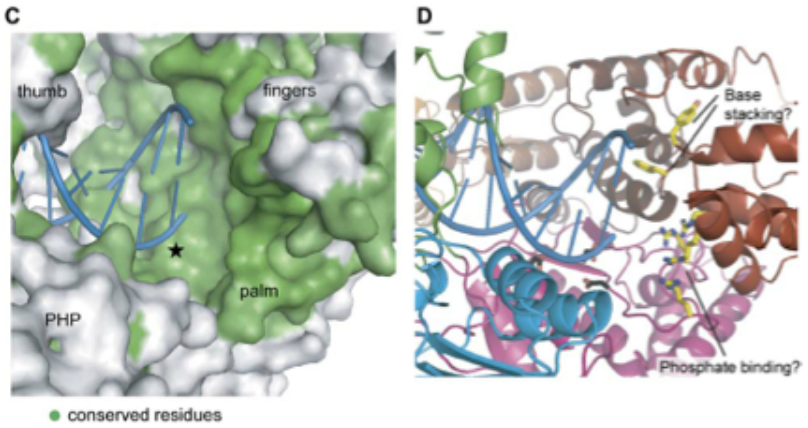


Figure 5. Model for DNA Binding in Pol III

(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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PIXELS AND MORE

P protein Ph1877p from hyperthermophilic archaeon Pyrococcus horikoshii OT3. Biochem. Biophys. Res. Commun. *319*, 787–794.

Teplyakov, A., Obmolova, G., Khil, P.P., Howard, A.J., Camerini-Otero, R.D., and Gilliland, G.L. (2003). Crystal structure of the Escherichia coli YcdX protein reveals a trinuclear zinc active site. Proteins *51*, 315–318.

Terwilliger, T.C. (2000). Maximum-likelihood density modification. Acta Crystallogr. D Biol. Crystallogr. *56*, 965–972.

Theobald, D.L., Mitton-Fry, R.M., and Wuttke, D.S. (2003). Nucleic acid recognition by OB-fold proteins. Annu. Rev. Biophys. Biomol. Struct. *32*, 115–133.

Waga, S., and Stillman, B. (1998). The DNA replication fork in eukaryotic cells. Annu. Rev. Biochem. *67*, 721–751.

Wang, J., Sattar, A.K., Wang, C.C., Karam, J.D., Konigsberg, W.H., and Steitz, T.A. (1997). Crystal structure of a pol alpha family replication DNA polymerase from bacteriophage RB69. Cell *89*, 1087–1099.

Wieczorek, A., and McHenry, C.S. (2006). The NH2-terminal php domain of the alpha subunit of the Escherichia coli replicase binds the epsilon proofreading subunit. J. Biol. Chem. *281*, 12561–12567.

Winn, M.D., Isupov, M.N., and Murshudov, G.N. (2001). Use of TLS parameters to model anisotropic displacements in macromolecular refinement. Acta Crystallogr. D Biol. Crystallogr. *57*, 122–133.

Yamagata, A., Kakuta, Y., Masui, R., and Fukuyama, K. (2002). The crystal structure of exonuclease RecJ bound to Mn2+ ion suggests how its characteristic motifs are involved in exonuclease activity. Proc. Natl. Acad. Sci. USA *99*, 5908–5912.

Yao, N., Leu, F.P., Anjelkovic, J., Turner, J., and O'Donnell, M. (2000). DNA structure requirements for the Escherichia coli gamma complex clamp loader and DNA polymerase III holoenzyme. J. Biol. Chem. *275*, 11440–11450.

Zhao, Y., Jeruzalmi, D., Moarefi, I., Leighton, L., Lasken, R., and Kuriyan, J. (1999). Crystal structure of an archaebacterial DNA polymerase. Structure *7*, 1189–1199.

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

FR (vector)

FR (tiff)

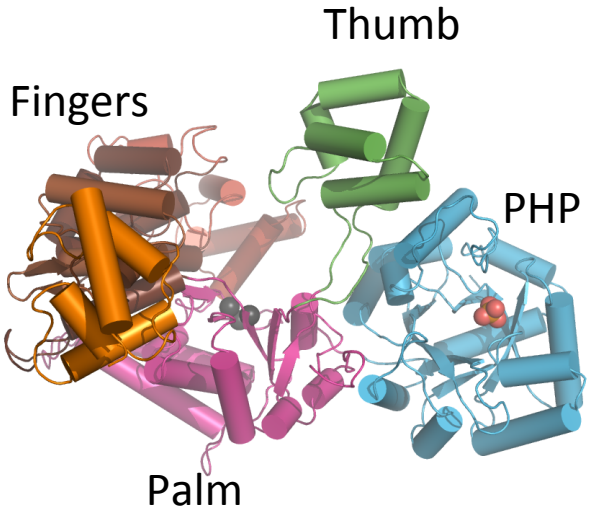
FR (png)

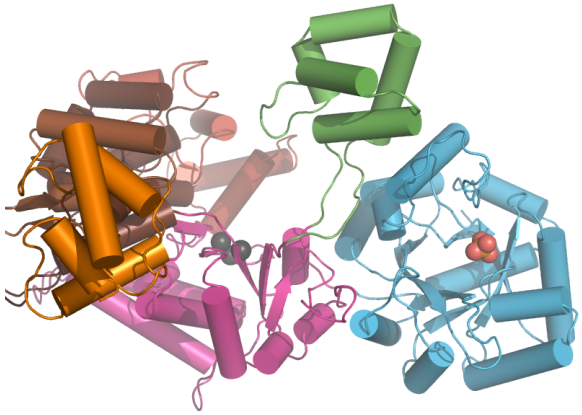
FR (jpeg)

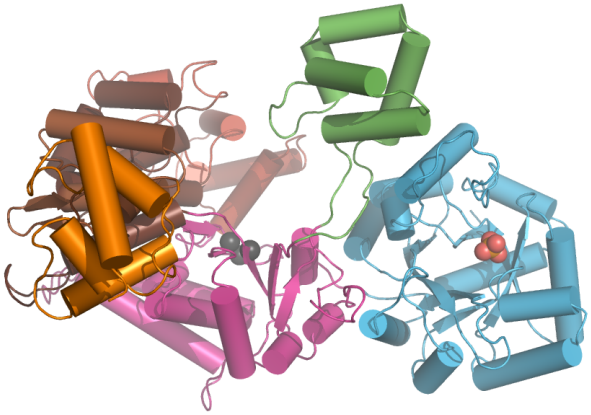
Vector
Illustrator
Powerpoint
Canvas
Coreldraw
InkScape

Pixel (bitmap)
Photoshop
Gimp
iPhoto
….

Representation & labeling



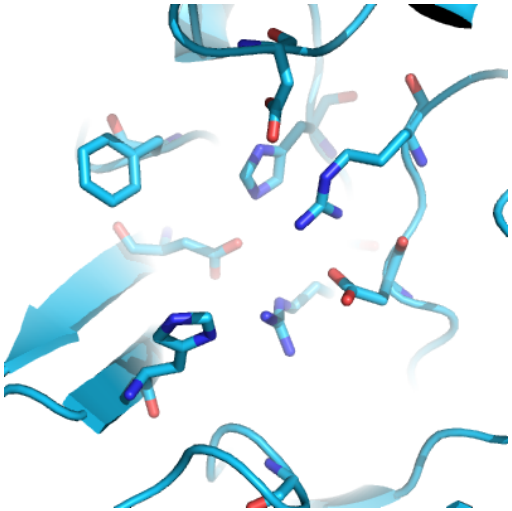


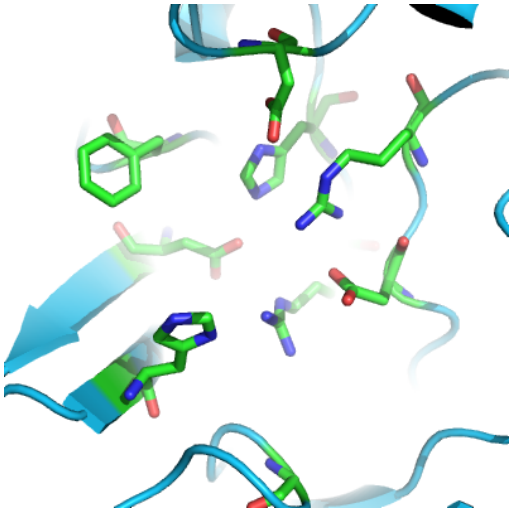


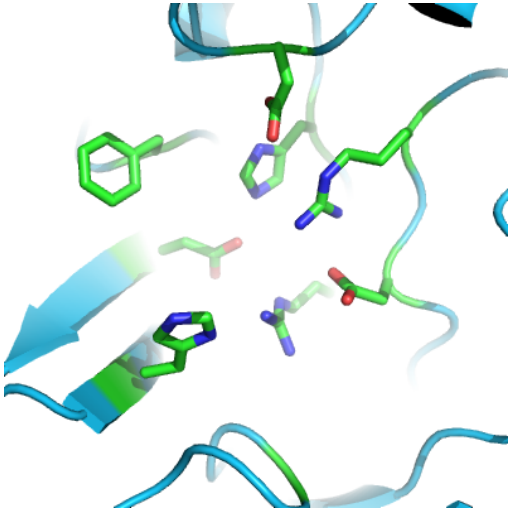
PHP domain
Palm domain
Thumb domain
Fingers domain

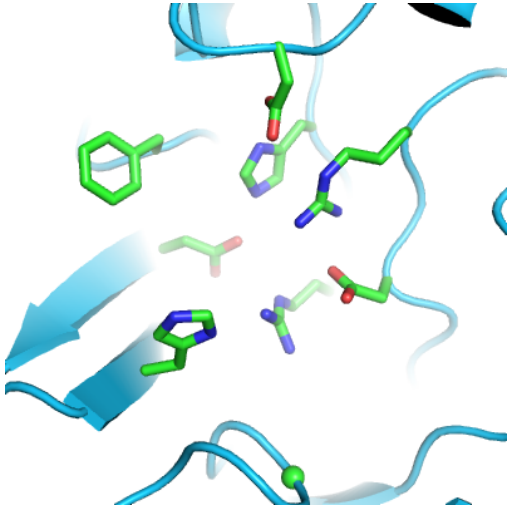
PHP domain (cyan), thumb domain (green), palm domain (magenta), Fingers domain (red/brown)

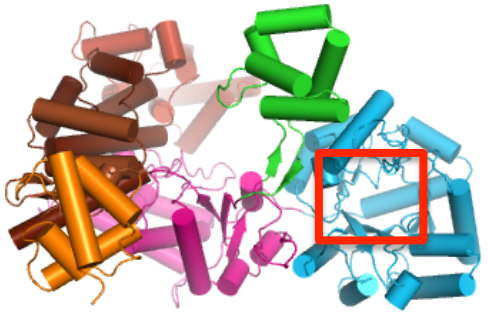
Representation & labeling



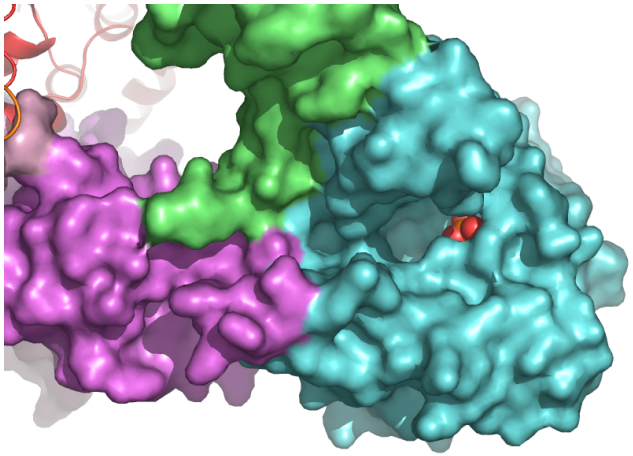






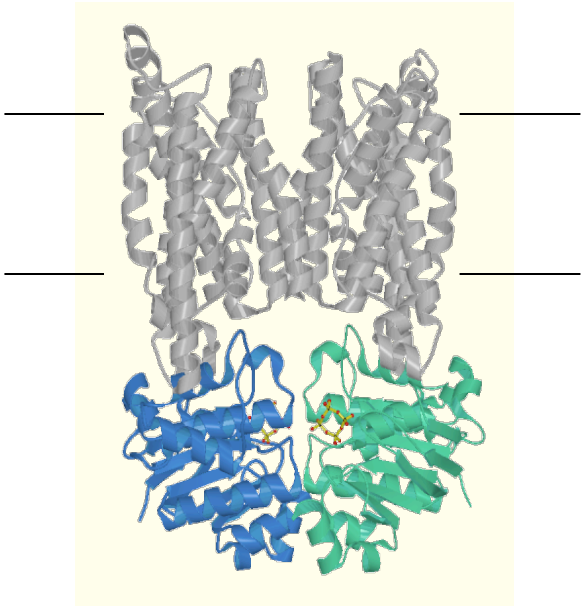


For side chains create a separate object
Don't show mainchain
Don't do fancy intros…..
No shadows



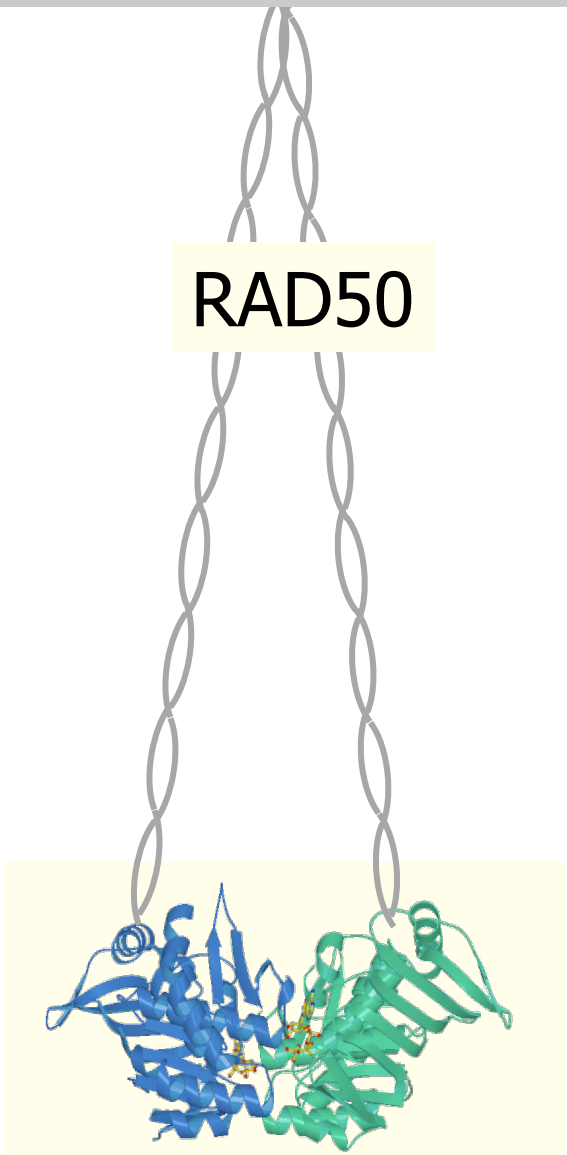
Representation & labeling

BtuCD



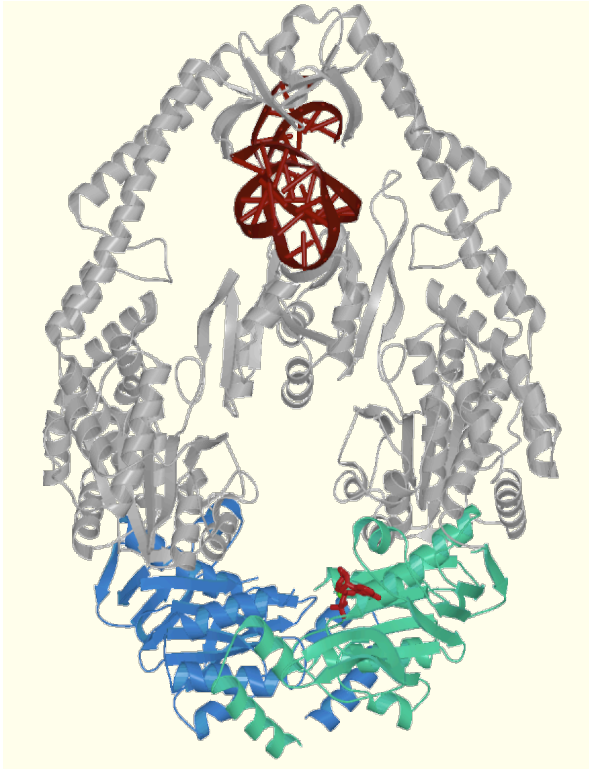
Vitamin B12 transport

RAD50



Double strand break repair

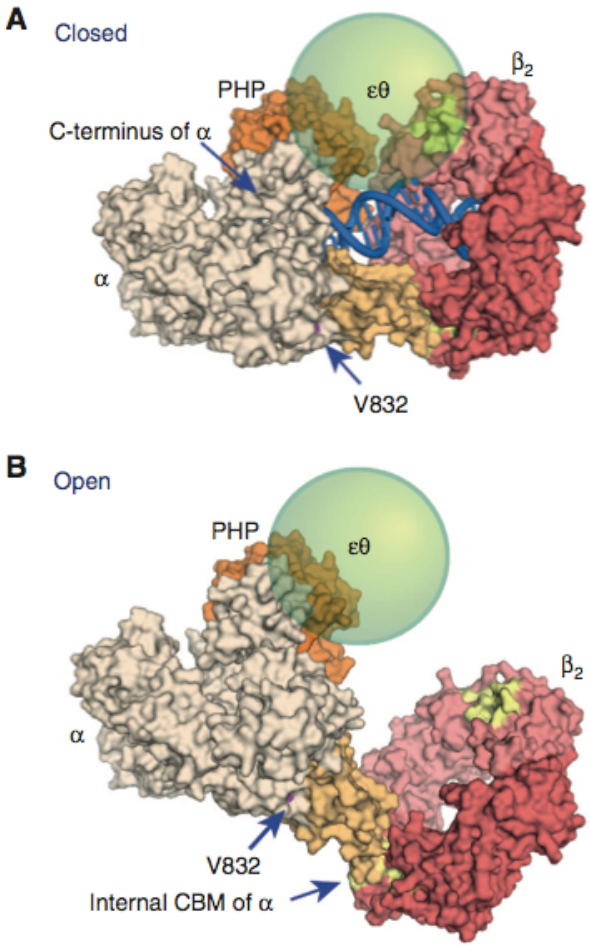
MutS

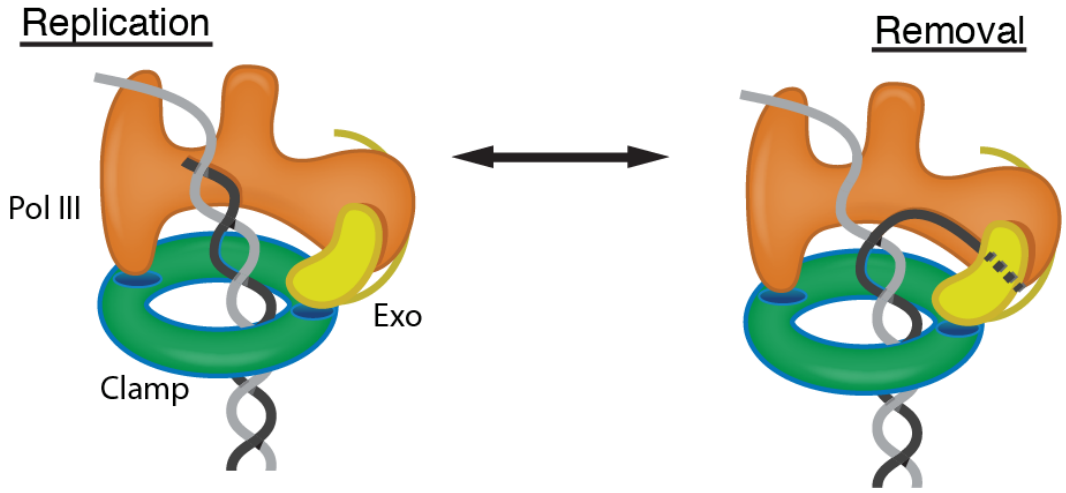


Mismatch repair

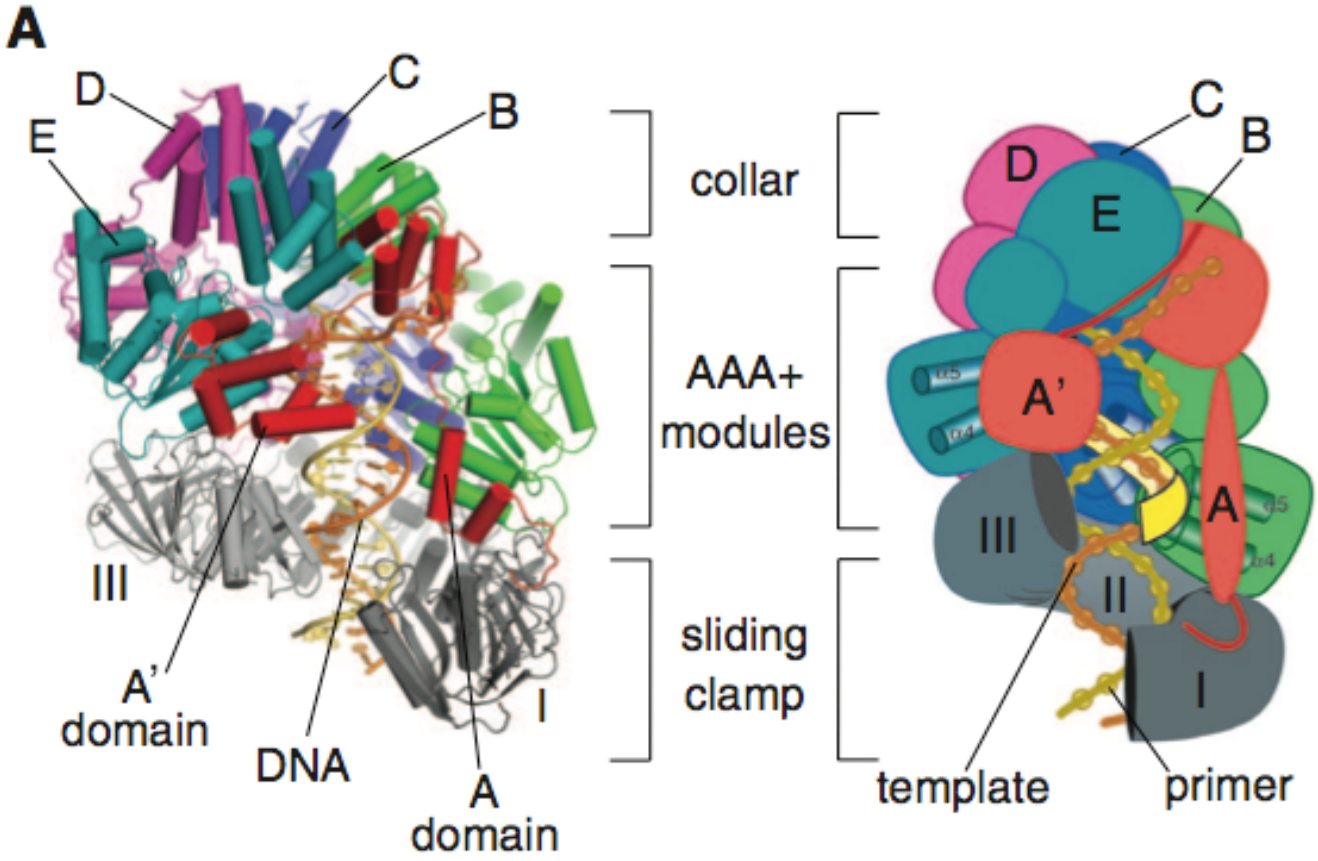
Getting the message across

How much detail?

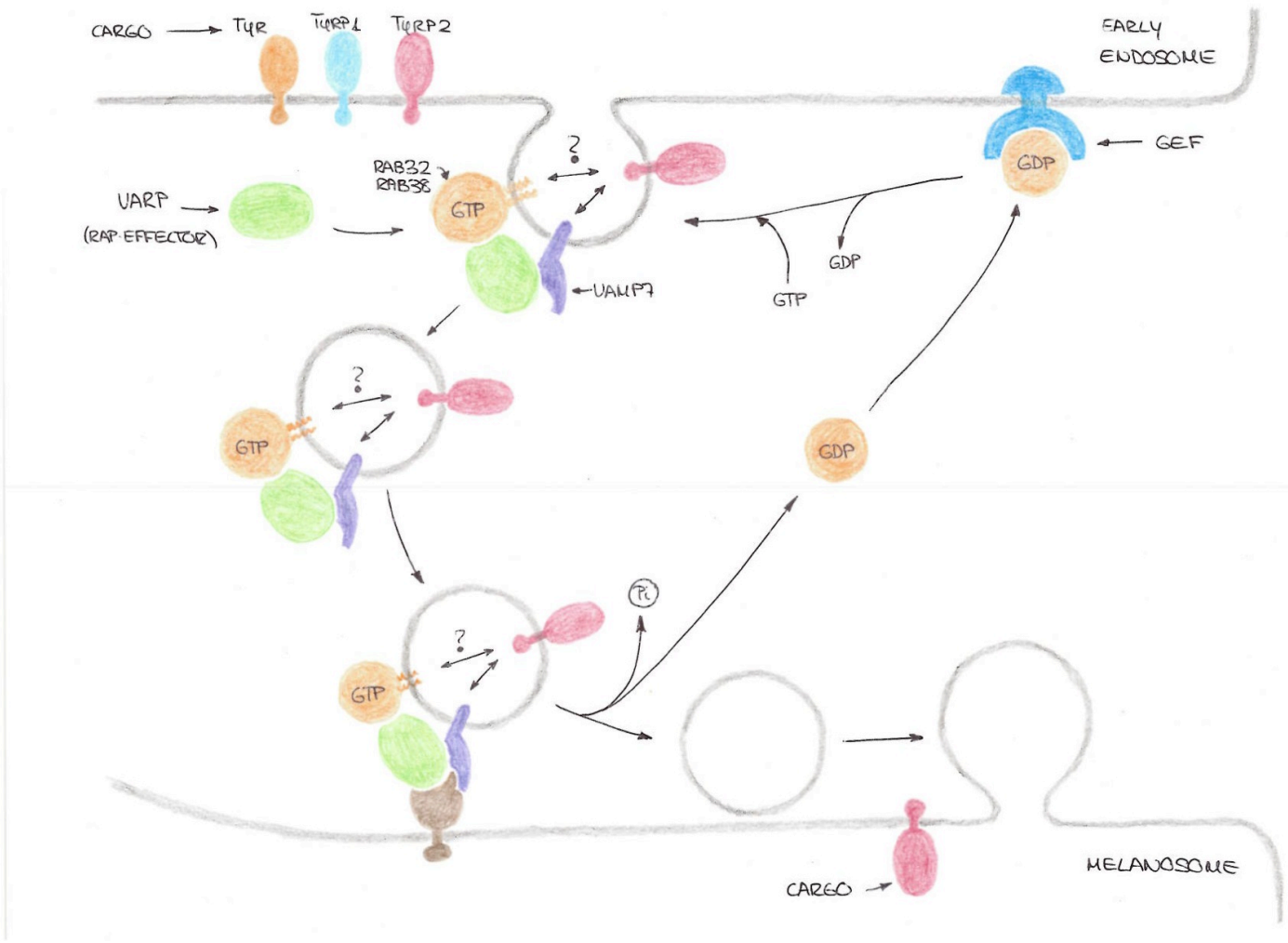




Getting the message across

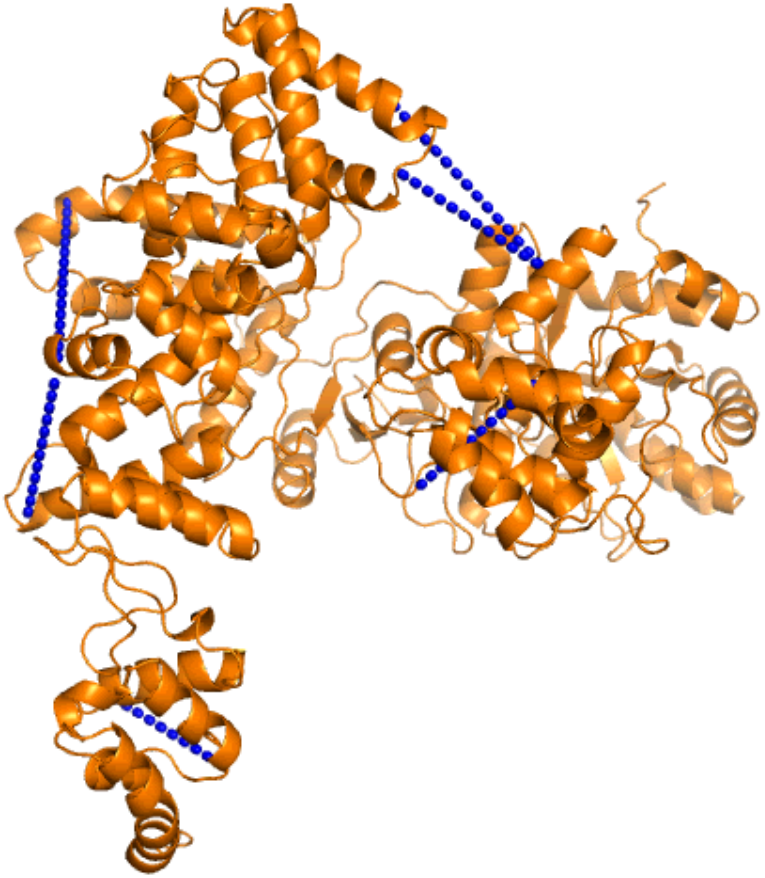


Getting the message across

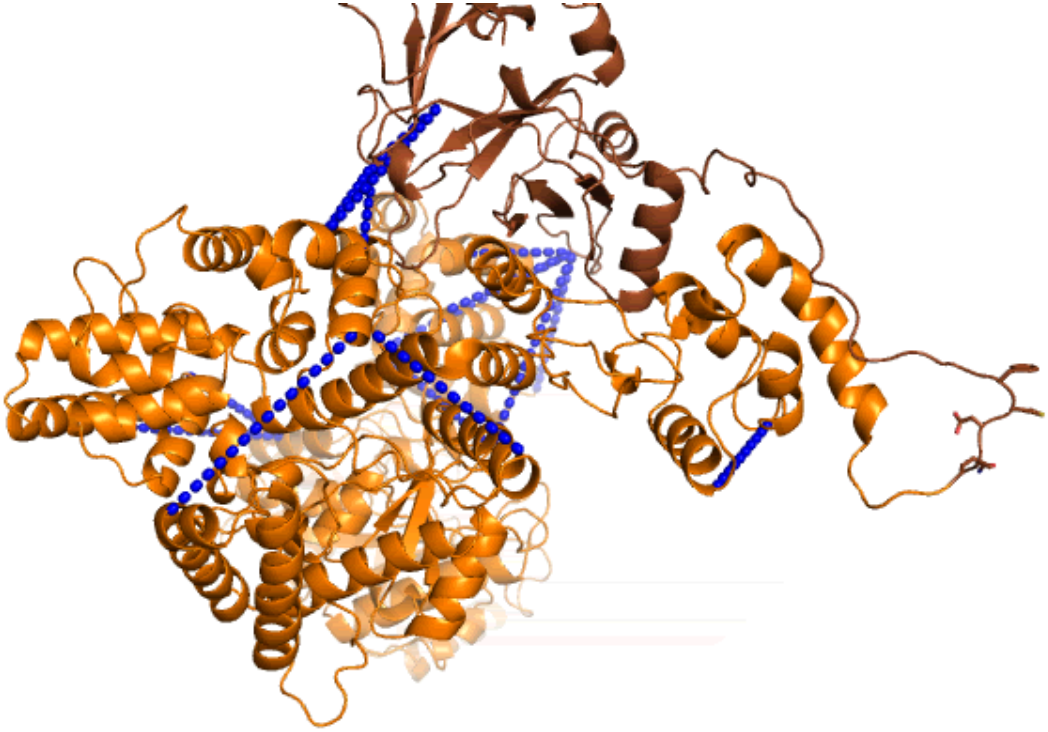


Inma Dorado

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…