# Do colors have a structure?

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#### Are the 5-type chromatin colors structurally different?







#### Derivation of the 5-type chromatin color

Filion et al. (2010). Cell, 143(2), 212-224



**Principal Component Analysis** 





#### Derivation of the 5-type chromatin colors

Filion et al. (2010). Cell, 143(2), 212-224



Position on chr2L (kb)

#### Are chromatin colors functional domains?

Hou et al. (2012). Molecular Cell, 48(3), 471–484



#### Percentage of chromatin surrounding TAD borders





#### Are chromatin colors functional domains?

Hou et al. (2012). Molecular Cell, 48(3), 471-484







#### **Resolution gap**

Marti-Renom, M. A. & Mirny, L. A. PLoS Comput Biol 7, e1002125 (2011)

Know	ledge								
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10 <sup>-10</sup>	10 <sup>-8</sup>	10 <sup>-6</sup>	10 <sup>-4</sup>	10 <sup>-2</sup>		10 <sup>0</sup>	10 <sup>2</sup>	10 <sup>3</sup>	S
								Resolution	1
10 <sup>-3</sup>			10 <sup>-2</sup>				10 <sup>-1</sup>	nesolution	μ





Hi-C technology

Lieberman-Aiden, E. et al. Science 326, 289–293 (2009) http://3dg.umassmed.edu





#### Structure determination using Hi-C data



# Biomolecular structure determination 2D-NOESY data



Chromosome structure determination 3C-based data



### **UCSF** The Integrative Modeling Platform framework

http://www.integrativemodeling.org Russel, D. et al. PLOS Biology 10, e1001244 (2012)



From Alber, F. et al. Nature 450, 695–701 (2007).



#### The four stages of integrative modeling





#### Representation

Constituent parts of the molecule







#### Representation

Constituent parts of the molecule





#### 3D modeling of the 5-type chromatin colors

Filion et al. (2010). Cell, 143(2), 212-224



Position on chr2L (kb)

#### Structural properties

50 1Mb regions. 10 enriched for each color





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#### Structural properties

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#### Structural features of the 5-colors



#### The 5-type chromatin colors structurally different

**BLACK** 





















# Clusters models.cluster\_analysis\_dendrogram(color=True) # Interactions, angle and density per particle models.interactions(cutoff=2000) models.walking\_angle(steps=(3, 5, 7), signed=False) models.density\_plot() # Plot the distance distributions between particles 13 and 30 in the top 100 models models.median\_3d\_dist(13, 30, models=range(100))





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http://gtpb.igc.gulbenkian.pt



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