

# Structure Analysis

**Talk to a Teacher**

**<http://spoken-tutorial.org>**

**National Mission on Education through ICT**

**<http://sakshat.ac.in>**

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**5 May 2016**



# Learning Objectives



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- ▶ **Measure distance between atoms in the structure**



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- ▶ Measure distance between atoms in the structure
- ▶ Show Hydrogen bonds
- ▶ Identify non-polar interactions
- ▶ Rotate bonds in the residues to get different rotamers



# Pre-requisites



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- **Chimera interface**





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- ▶ **Chimera interface**
- ▶ <http://spoken-tutorial.org>



# System Requirement



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- ▶ **Ubuntu OS version 14.04**



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- ▶ **Working internet connection**



# Hydrogen Bond Distances



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- ▶ **2.2 Å to 2.5 Å - Strong**





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- ▶ **2.5 Å to 3.2 Å - Moderate**



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- ▶ 2.2 Å to 2.5 Å - Strong
- ▶ 2.5 Å to 3.2 Å - Moderate
- ▶ 3.2 Å to 4.0 Å - Weak



# Clashes and Contacts



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- ▶ **Clashes** - Unfavorable interactions where atoms are too close together



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- ▶ **Clashes** - Unfavorable interactions where atoms are too close together
- ▶ **Contacts**- All direct interactions: polar and non-polar, favorable and unfavorable (including clashes)



# Summary



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- ▶ Measure distance between atoms in the structure
- ▶ Show Hydrogen bonds
- ▶ Identify non-polar interactions
- ▶ Rotate bonds in the residues to find clashes and contacts
- ▶ Compare different rotamers



# Assignment





# Assignment

- ▶ Open a structure of Squalene Synthase (pdb code: **3w7f**)
- ▶ Rotate bonds in **Tyr 41** residue to determine Clashes and Contacts
- ▶ Compare the rotamers



# About the Spoken Tutorial Project

- ▶ Watch the video available at [http://spoken-tutorial.org/What\\_is\\_a\\_Spoken\\_Tutorial](http://spoken-tutorial.org/What_is_a_Spoken_Tutorial)
- ▶ It summarises the Spoken Tutorial project



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- ▶ It summarises the Spoken Tutorial project
- ▶ If you do not have good bandwidth, you can download and watch it



# Spoken Tutorial Workshops

## The Spoken Tutorial Project Team

- ▶ Conducts workshops using spoken tutorials
- ▶ Gives certificates to those who pass an online test
- ▶ For more details, please write to [contact@spoken-tutorial.org](mailto:contact@spoken-tutorial.org)



# Acknowledgements

- ▶ Spoken Tutorial Project is a part of the Talk to a Teacher project
- ▶ It is supported by the National Mission on Education through ICT, MHRD, Government of India
- ▶ More information on this Mission is available at

<http://spoken-tutorial.org/NMEICT-Intro>

