

Structure Analysis

Talk to a Teacher

<http://spoken-tutorial.org>

National Mission on Education through ICT

<http://sakshat.ac.in>

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Learning Objectives



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



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- ▶ **Show Hydrogen bonds**



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- ▶ 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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Hydrogen Bond Distances

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- ▶ **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



Clashes and Contacts

- ▶ **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
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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



Acknowledgements

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- ▶ **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>

