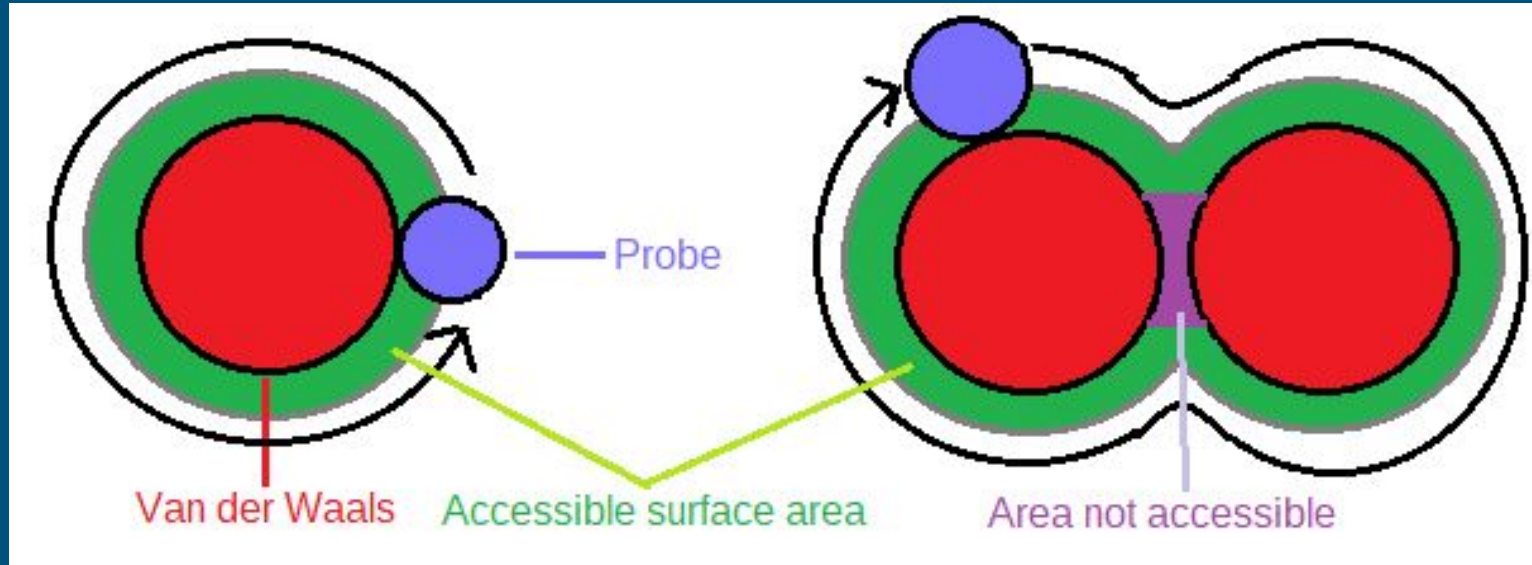


# Calculating the accessible surface area of a protein

By Bel Alexis  
2022-2023

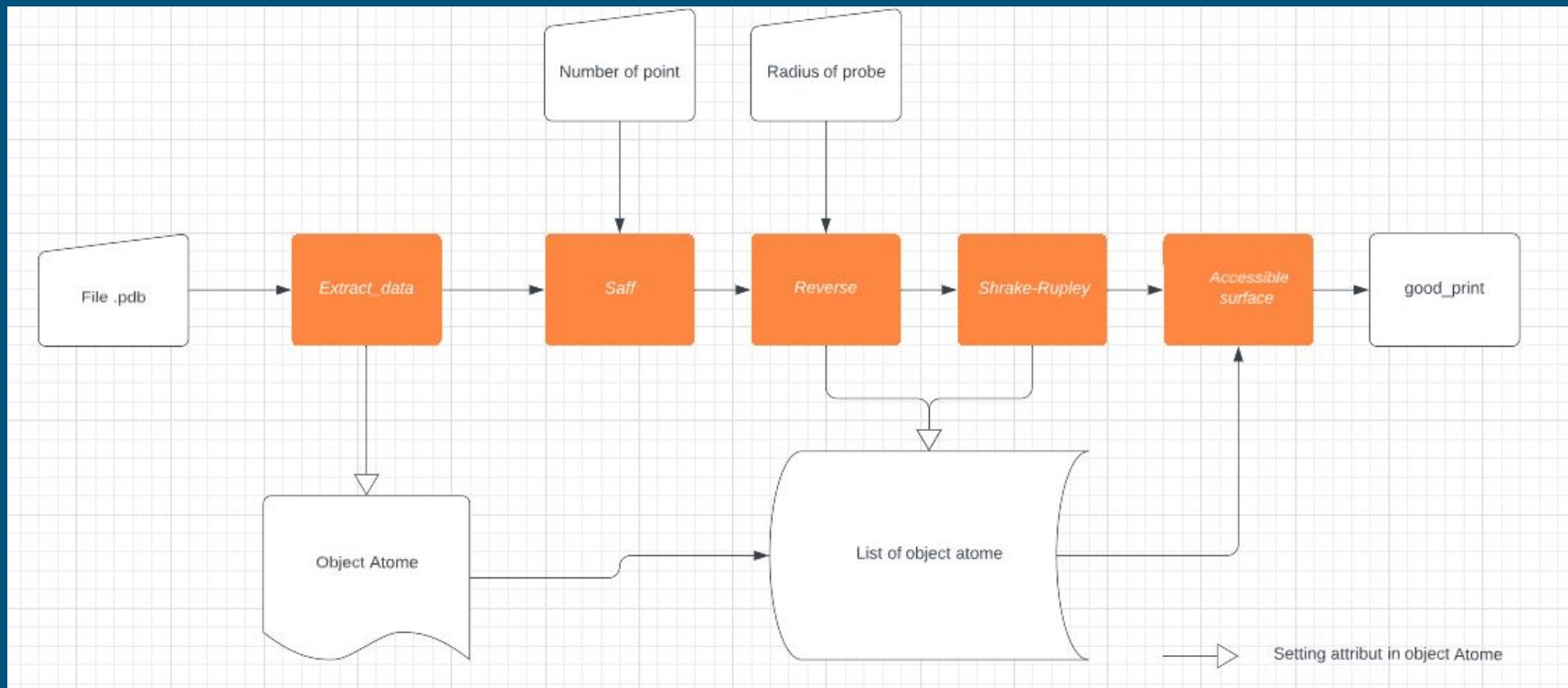
Shrake, A; Rupley, JA. (1973). "Environment and exposure to solvent of protein atoms. Lysozyme and insulin". J Mol Biol 79 (2): 351–71. doi: 10.1016/0022-2836(73)90011-9.

# What is ASA?



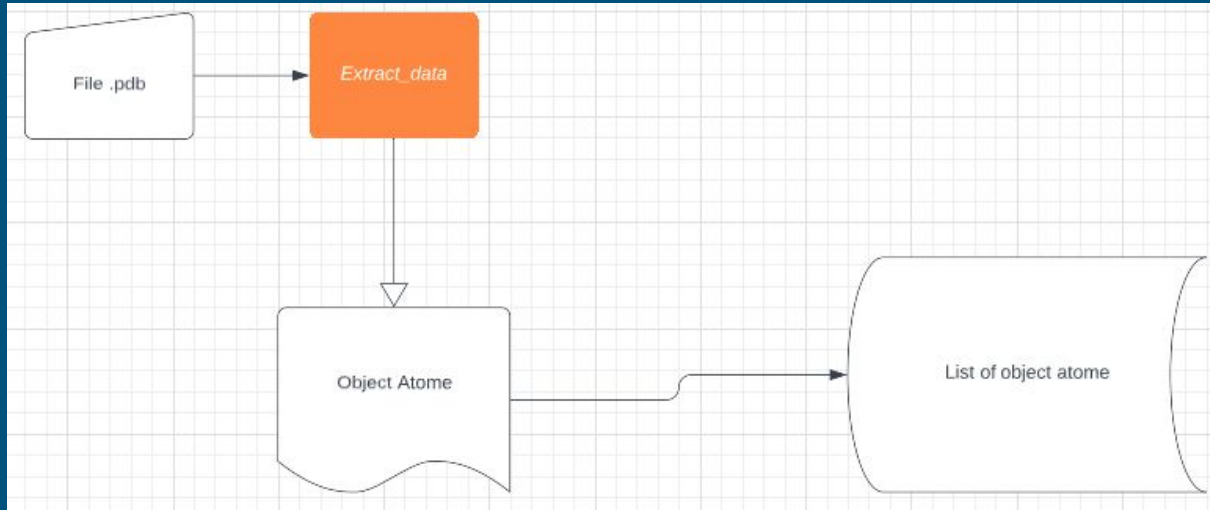
Picture of the algorithm of Shrake Rupley

# Pipeline



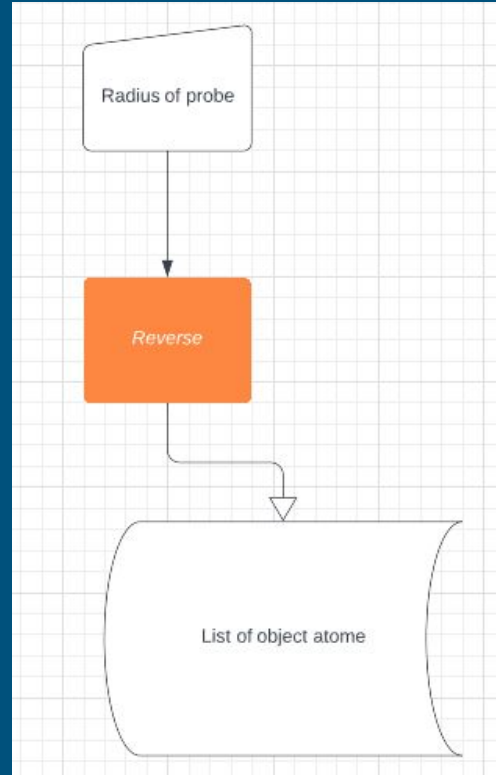
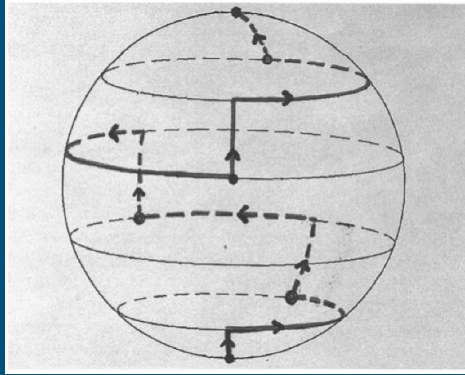
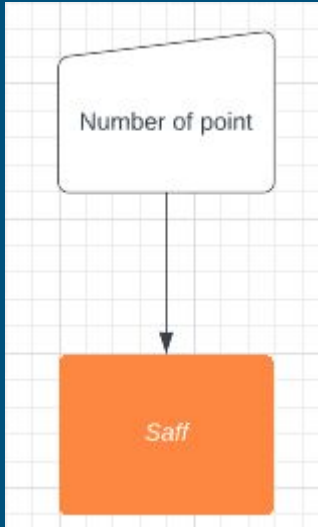
# Pipeline extraction

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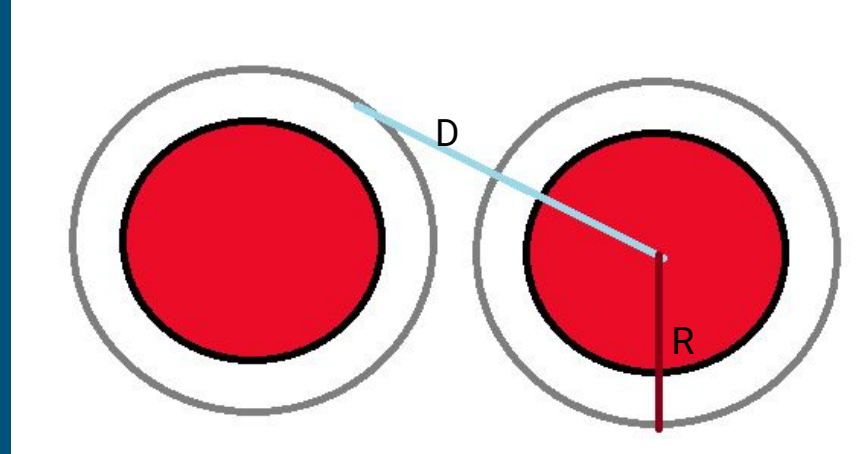
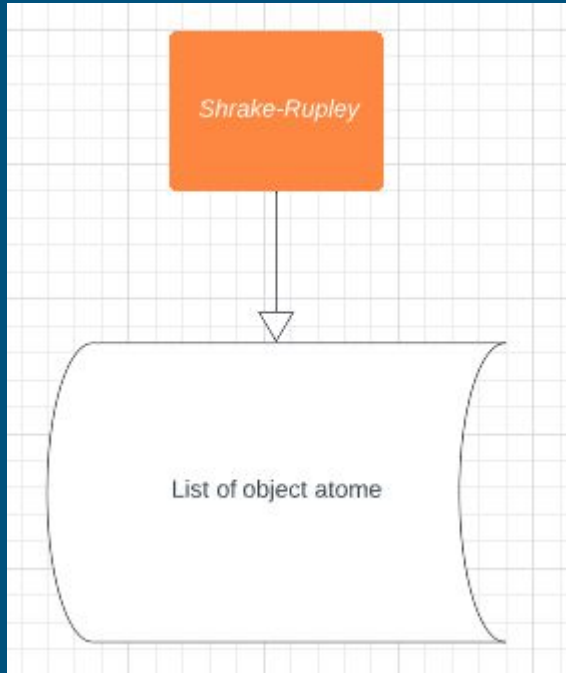
- Extract data from a .pdb
- For each atom a object atom is creates
- A list contain all the object atom

# Pipeline: Saff et reverse



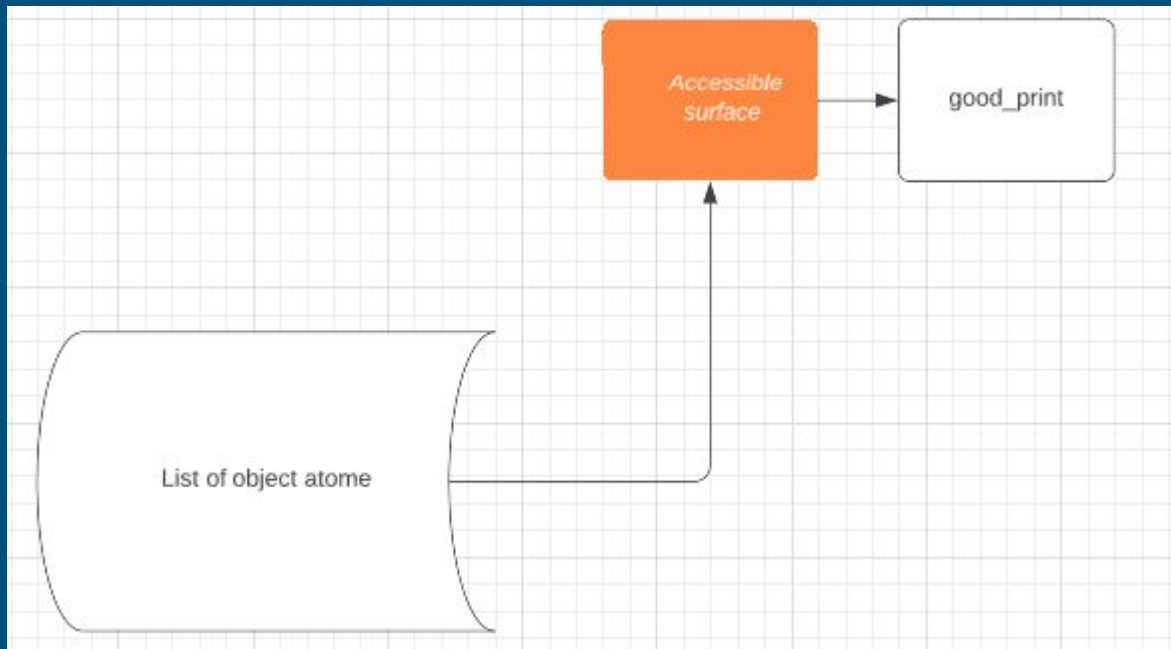
- Spherical coordinate to 3d coordinates
- 3d coordinates in object atom

# Pipeline: Shrake Rupley



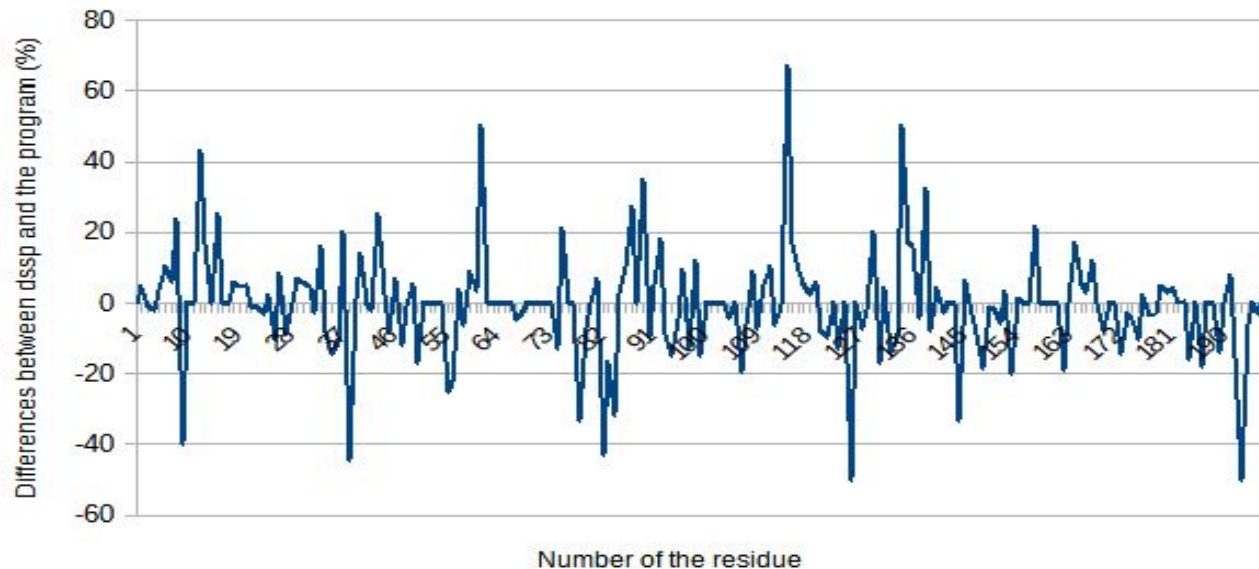
Compare D and R to determine if a point is buried or not

# Pipeline: Accessible surface



- Add the ASA of atom by residue
- Add the ASA of All residue
- Add the maxASA of all residue
- Ratio of Sum of ASA / Sum MaxASA

# Result:



Mean of the differences : -0.3%  
Script = 9730 A<sup>2</sup>  
DSSP = 9623 A<sup>2</sup>

28 % of the protein is accessible

Difference between the results obtain by dssp and by the program



# Discussion:

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- Working program
- Testing on larger protein
- Multiprocessing



Thank you for your attention