

BIN515 Assignment 2

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Q2)

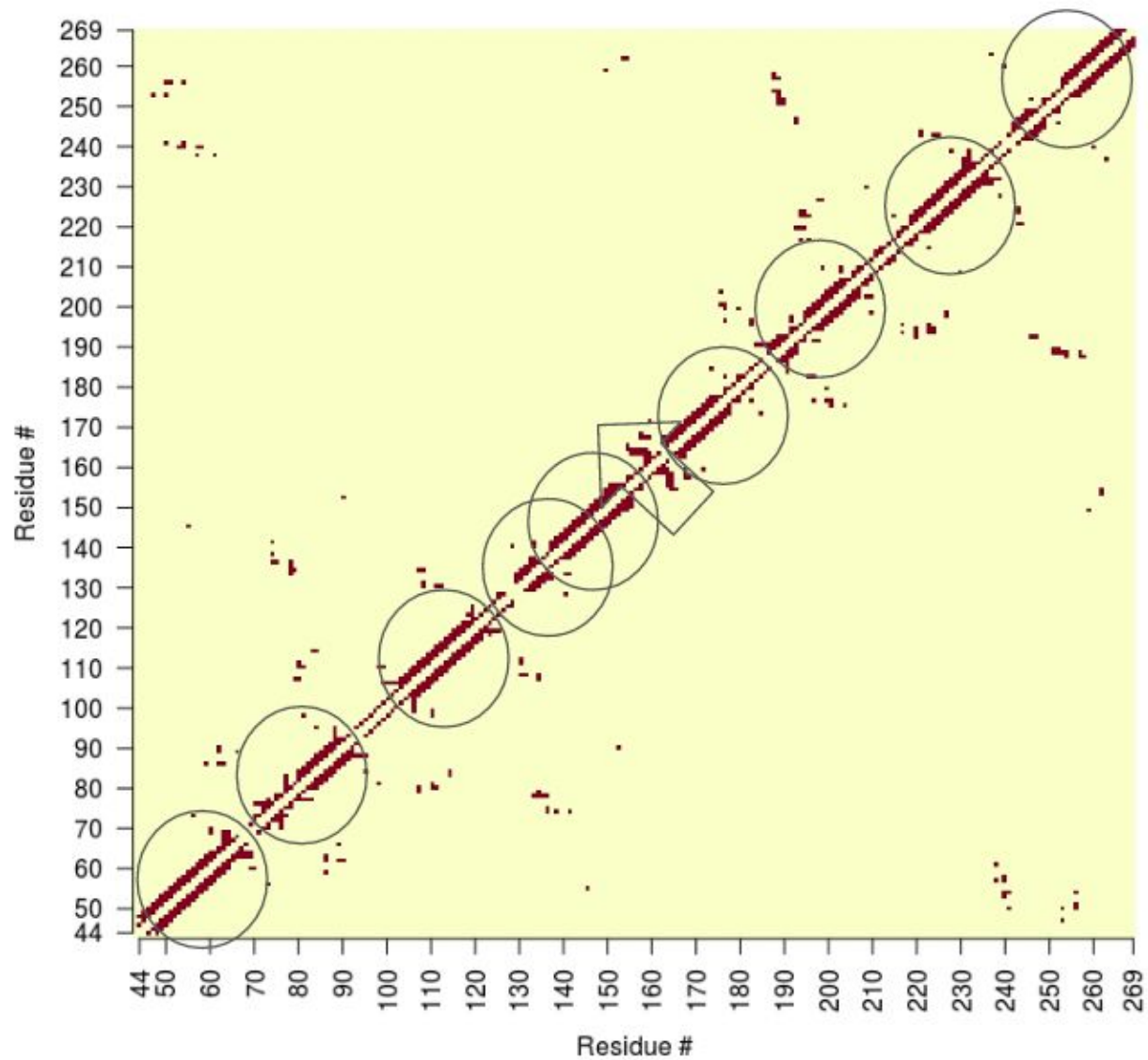


Fig1: Contact map of protein with PDB ID 6o31.

In Fig1, encircled structures are α -helices and arrow is parallel B-sheet

Q3)

- a) Residue 111, 168 and 223 are the ones that has most connection
- b) Residue 134, 155, 164, 177, 189, 224, 232, 111, 168 and 223 are the 10 residues that have the most connection.

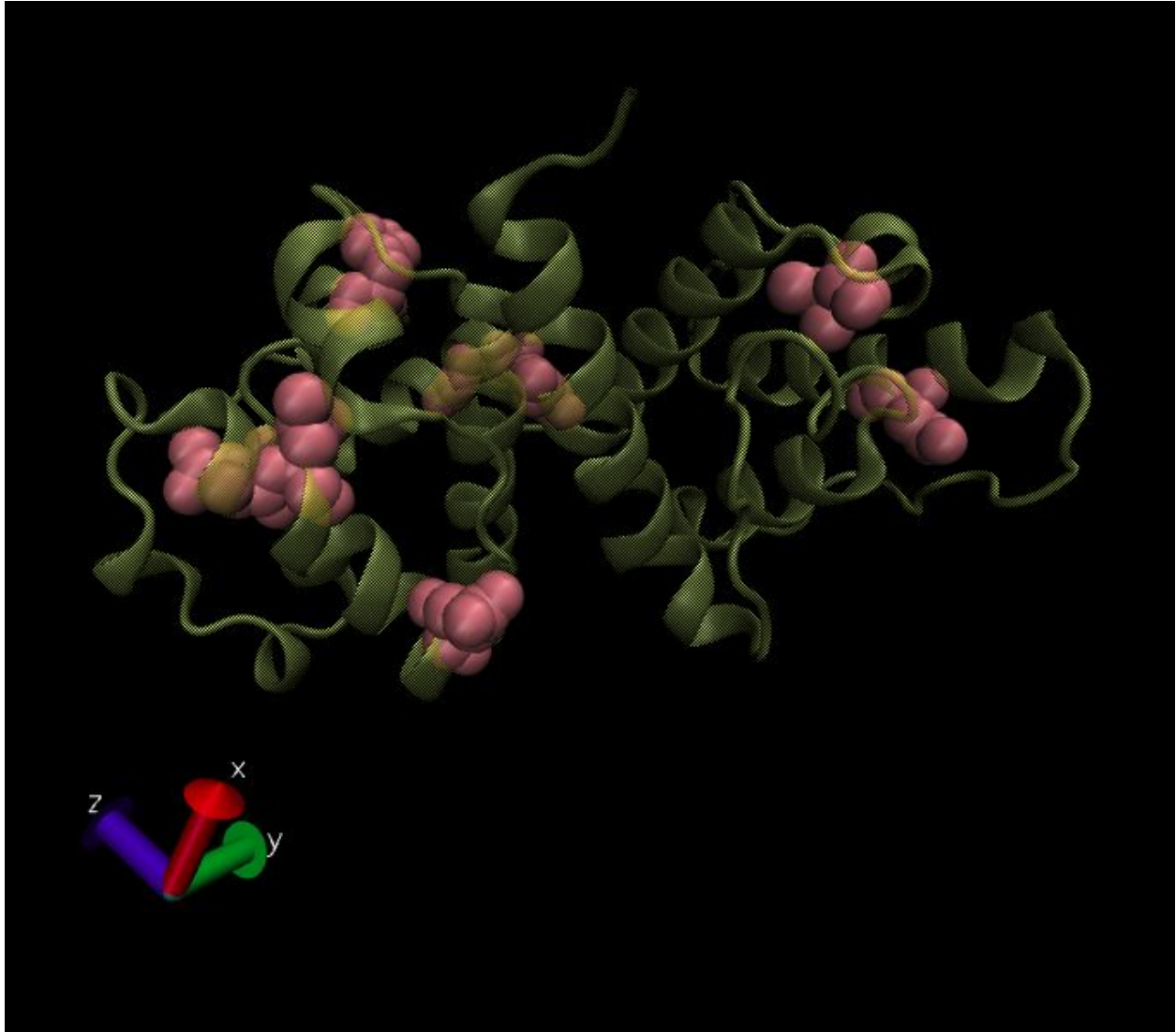


Fig2: Protein representation in newcartoon and 10 most connected residues representation of van der waals.

Just by checking visually, the connected residues are mostly in the core region.

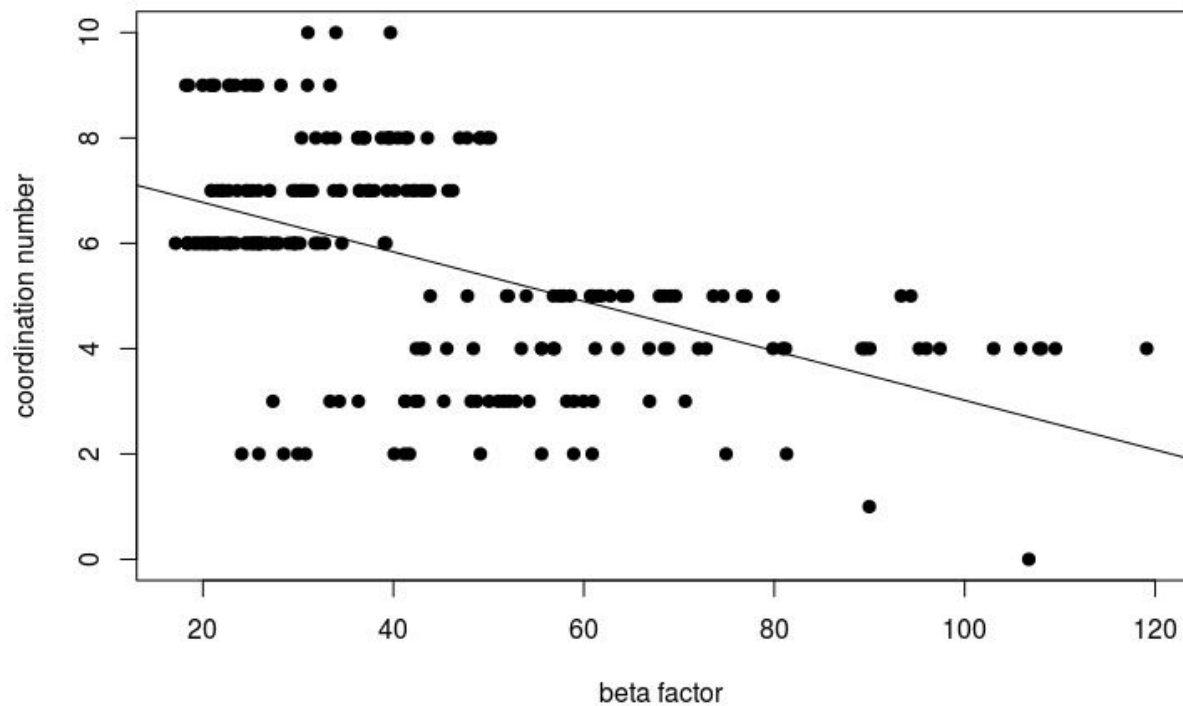


Fig3: Scatter plot of coordination number vs B-factor 6o31.

- c) In Fig3. there seems to be a negative correlation between B-factor and coordination number. This negative correlation may be due to the flexibility of the residues. The more contacted residues, the less flexible they are.

Q4)

- b) Since the sum of the all the coordinates is 10^{-12} , the new coordinates satisfy the condition.

Q5) 10 models are available for 6u3r.

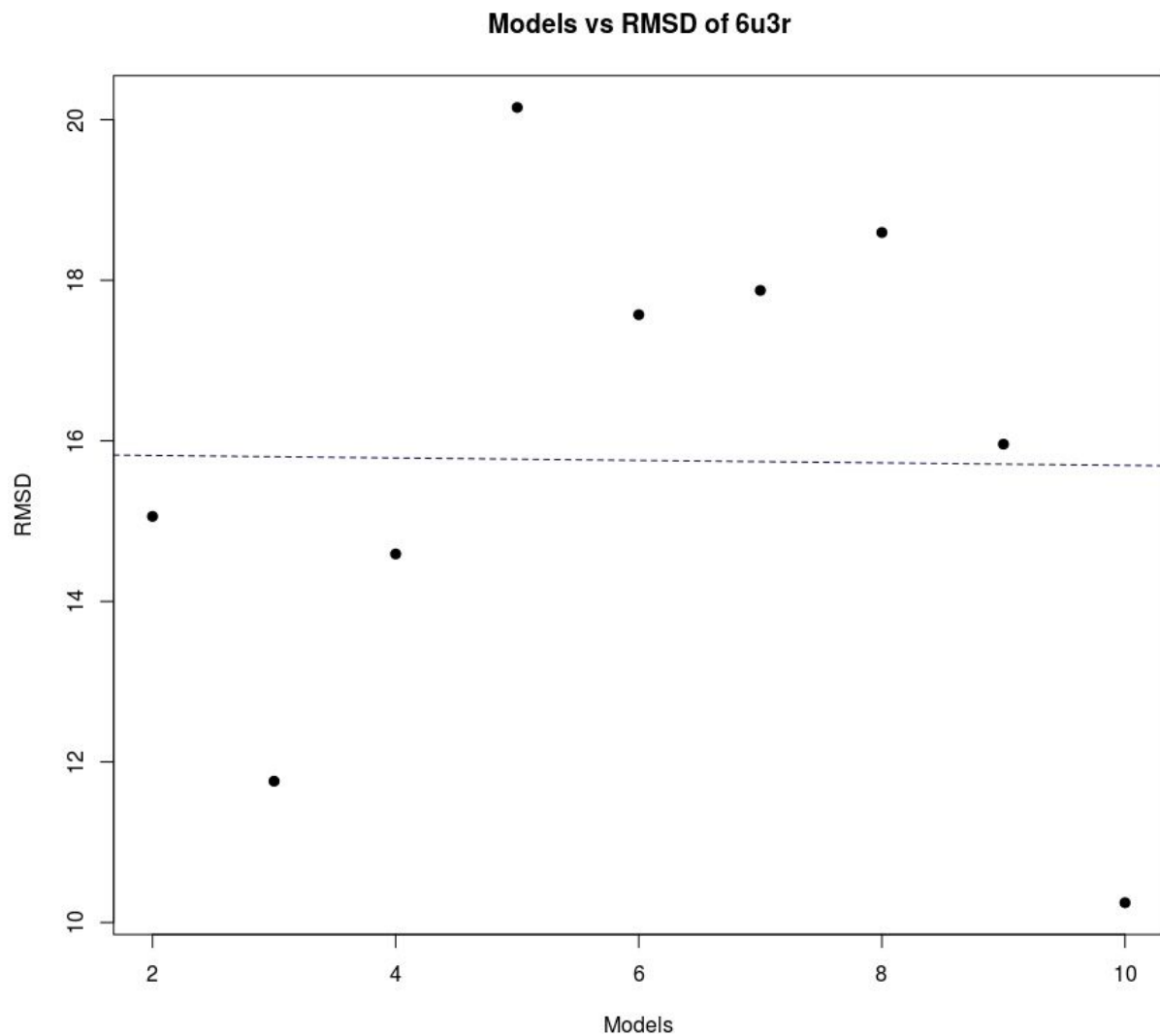


Fig4: Scatter plot of RMSD vs 1st model vs the rest of the models.

There seems to be no correlation between RMSD of the models. In our case, if each model were different proteins, we could assume that they were not similar since their RMSD values are too high. But in this situation we could assume that the protein is very flexible.

Q6)

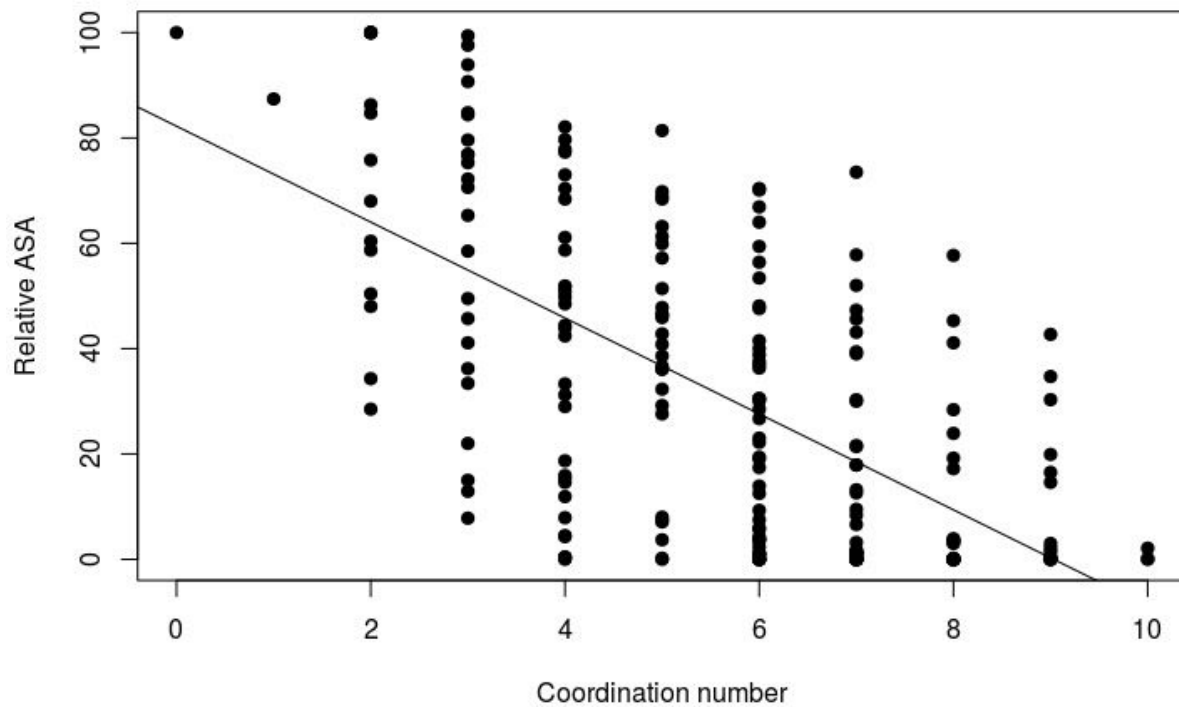


Fig5: Relationship between accesible surface area vs coordination number of residues.

The Pearson Correlation test revealed that there is a strong negative correlation between above 2 variables with correlation coefficient of -0.62 and p-val less than $10e-16$. This indicates that residues with more contacts tend to be in the core of the protein, not on the surface.

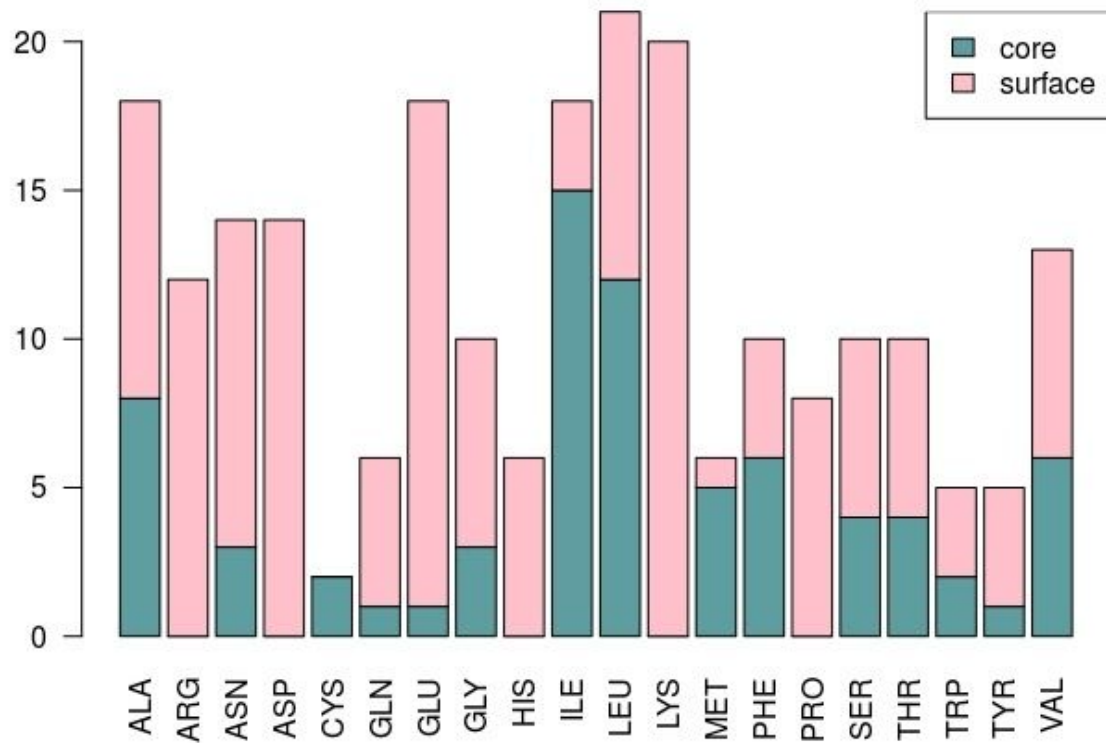


Fig6: Distribution of core vs surface residues across different amino acids.

c) Leucine and Isoleucine are good examples of aminoacids being predominantly in the core of the protein whereas aspartate, histidine, arginine, lysine and glutamate are the good examples of surface residues since they are charged amino acids.