Result & Discussion :-

For the Selected query the bond distance between the selected atoms was found to be. ε LU194 & OE2 was 5.38

*) The bond angle of selected atoms was LEU34 - CD1 - ARG11 was 5.12°

*) Atom selected psi, phi, ω angles were -67.56°, -41.36°, -178.59°

*) The torsion angles were also adjusted such that angles were fit in the allowed regions of ramachandran plot.

*) Tools such as color, display & align were used to study the molecules.

*) The active site analysis carried out helped in the understanding of the ability of protein to bind to ligand molecules, thus helping in understanding of the proteins conformational changes.

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*) Click select all menu & wind & ramachandran plot to display ramachandran plot.

*) Energy minimisation can be done by clicking on select option & select all.

*) Click on tool & select energy minimisation option.

*) A window opens check for all values to be in negative. then save new minimised protein.

*) loop can be introduced in protein molecule by selecting built loop & built option.

*) By selecting atleast 3 points on molecules to introduce looping.

*) Select & open the downloaded legand molecule in the same window & study the superimposed protein with respect to structural alignment & compare the active site.

Analysis of Active site

Query :- 1LDM

1) Open the PDB file 1LDM. select the compute H-bond item of tool menus.

2) Click on control panel window scroll to the bottom & select the groups NADOXM. they should turn red. Now Choose the item shows only H bond from selection on the display menu, then choose the items shows only group with visible H-bonds & same menu.

*) Finally hit = key of numerical key pad & to rescale & recentre view.

Query: 1Q2R / 1LDM

URL: https://www.expasy.org/SPDBV/
https://www.rcsb.org.

Procedure:-

* Login PDB database using www.rcsb.org
* In the search box type the given query ID & download the protein in PDB format.
* Open SPDBV that is installed in your system.
* Select file & open the downloaded query in PDB format.
* To manipulate the molecule Click on tool & select relevant tool for zooming & rotating it.
* To visualise the structure in 3D Select display option & Seled render in solid 3-D.
* To display colour Click secondary structure by default and indicates α-helix, Yellow β-sheet.
* Click 5th button in tool bar & Select two atoms on the molecule to Calculate bond length or distance between two atoms.
* Click 6th bottom in tool bar & seled 3 atoms to Calculate bond angle or radius between 3 atoms.
* Click 7th button in tool & Select 4 atoms to Calculate dihydral [Torsion] angle between 4 atoms.
* In control panel window Right Click Symbol &/ribbon to display protein structure in backbone ribbon model.

Determination of Ligand - protein interactions using SPDBV // SWISS

Aim:- To determine Ligand protein interaction by using SPDBV - Swiss Software tool.