ABSTRAK

ANALISIS DINAMIKA MOLEKUL PROTEIN *LYSOZYME* PUTIH TELUR DENGAN MODEL POTENSIAL LENNARD-JONES MENGGUNAKAN APLIKASI GROMACS

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Telah dilakukan analisis dinamika molekul protein lysozyme putih telur yang diselimuti air bentuk kubik dengan variasi temperatur 300 K, 325 K, dan 350 K serta melakukan perhitungan nilai energi potensial dengan persamaan Lennard Jones yang dilakukan dengan aplikasi Gromacs. Pada temperatur 300 K menunjukan nilai tekanan 2,54 bar dan nilai densitas 997,54 kg/m3 serta terjadi perubahan unfolded state di rantai asam amino ARG21-CA dan SER81-CA yang menghasilkan energi potensial 2992,14 kJ/mol. Pada temperatur 325 K menunjukan nilai tekanan 4,84 bar dan nilai densitas 974 kg/m3 serta terjadi perubahan unfolded state di rantai asam amino ASP101-CA dan GLN121-CA yang menghasilkan energi potensial 2994,55 kJ/mol. Pada temperatur 350 K menunjukan nilai tekanan 0,82 bar dan nilai densitas 948,747 kg/m3 serta terjadi perubahan unfolded state di rantai asam amino ARG21-CA dan menghilangnya rantai asam amino GLN121-CA yang menghasilkan energi potensial 2999,65 kJ/mol. Hasil Root Mean Standart Deviation (RMSD) menunjukan bahwa protein mulai terdenaturasi pada temperatur 350 K yang ditandai pemutusan rantai asam amino GLN121-CA sejauh 0.07 nm.

Kata kunci: dinamika molekul, Lennard-Jones, lysozyme, Gromacs.

ABSTRACT

THE MOLECULAR DYNAMICS ANALYSIS OF *LYSOZYME* PROTEIN EGG WHITE BY LENNARD-JONES POTENTIAL USING THE GROMACS APPLICATION

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The molecular dynamic analysis of lysozyme protein has been done using Gromacs application. Lysozyme protein filled by water in the cubic form with variation of temperature was 300 K, 325 K, and 350 K and calculated potential energy values used Lennard Jones equation. Structure protein on temperature was 300 K showed that pressure value was 2,54 bar and density value was 997,54 kg/m^3 then protein changed in unfolded state on ARG21-CA and SER81-CA amino acid chain with potential energy was 2992,14 kJ/mol . Structure protein on temperature was 325 K showed that pressure value was 4,84 bar and density value was 974 kg/m^3 then protein changed in unfolded state on ASP101-CA and GLN121-CA amino acid chain with potential energy was 2994,55 kJ/mol. Structure protein on temperature was 350 K showed that pressure value was 0,82 bar and density value was 948,747 kg/m^3 then protein changed in unfolded state on ARG21-CA amino acid chain and lost on GLN121-CA amino acid chain with potential energy was 2999,65 kJ/mol. Root Mean Standard Deviation (RMSD) showed that the protein will be denaturated on temperature 350 K caused by lost on GLN121-CA amino acid with distance was 0.07 nm.

Keywords: *molecular dynamics, Lennard-Jones, lysozyme, Gromacs.*