Bab 5

SIMPULAN

5.1 Simpulan

Hasil pengolahan data menunjukkan nilai rata-rata RMSD untuk jarak periodik minimum 2.0 nm adalah 0.3149 nm paling kecil bila dibandingkan dengan nilai rata-rata RMSD untuk jarak 1.6 nm yaitu 0.3247 nm dan nilai rata-rata RMSD untuk jarak minimum periodik 2.4 nm yaitu 0.3302 nm, nilai RMSF backbone protein lebih kecil dibandingkan atom penyusun lain nya ini menunjukkan backbone protein lebih rigid dibanding atom penyusun lain nya. Nilai jari – jari girasi yang paling kecil ditunjukkan oleh protein Argonaute dengan jarak minimum periodik 2.0 nm, ini menunjukkan molekul protein Argonaute semakin kompak. Nilai *Solvent accessible Surface* paling besar ditunjukkan pada jarak minimum periodik 2.0 nm.

Berdasarkan hasil pengolahan data, dapat disimpulkan bahwa bahwa tidak ada perbedaan bermakna pada ketiga simulasi selama 5000 ps.

Dapat disarankan untuk simulasi dapat digunakan jarak antar molekul bayangan cermin 1.6 nm.

5.2 Alur Penelitian Selanjutnya

1. Perlu adanya penelitian lebih lanjut pada temperatur yang berbeda.
2. Perlu adanya penelitian lebih lanjut pada tekanan yang berbeda.

DAFTAR PUSTAKA

Berendsen, J.H.C., D. van der Spoel, R. Van Drunen, 1984, Molecular dynamics with coupling to an external bath, **J Chem Phys.,** 81, 3684-3690.

Brooks, B.R., R.E. Bruccoleri, B.D. Olafson, D.J. States, S. Swaminathan, M. Karplus, 1982, CHARMM : a program for macromolecular energy, minimization, and dynamics calculations, **J Comput Chem.,** 4, 187-217.

Couzin, J ., 2002, Small RNAs Make Big Splash, **Sciencemag.**, 298, 2296-2297.

Darden, T., D. York, L. Pedersen, 1993, Particle mesh Ewald: an N. Log (N) method for Ewald sums in large system, **J Chem Phys.,** 98, 10089-10092.

Elbashir, S. M., Harborth, J., Lendeckel, W., Yalcin, A., Weber, K. and Tuschl, T., 2001, Duplexes of 21-nucleotide RNAs mediate RNA interference in mammalian cell culture, **Nature,** 411, 494-498.

Frenkel, D., B. Smit, 2002, **Understanding molecular simulation: from algorithms to applications**, USA: Academic Press., Sandiego, California.

Harvey, S.C., 1989, Treatment of electrostatic effect in macromolecular modelling, **Proteins: struct func gen.,** 5, 78-92.

Höck, J., G. Meister, 2008, The Argonaute Protein Family, **Genome biology.,** 9, 210.

Ikeda, K., M. Satoh, K. M.Pauley, M. J. Fritzler, W. H. Reeves, E. K. L. Chan, 2006, Detection of the Argonaute Protein Ago2 and microRNAs in the RNA Induced Silencing Complex (RISC) Using a MonoclonalAntibody, **J Immunol Methods.,** 317(1-2), 38–44.

Kuszewski, J., A.M. Gronenborn, G.M. Clore,1999, Improving the Packing and Accuracy of NMR Structures with a Pseudopotential for the Radius of Gyration, **J Am Chem Soc.,** 121, 2337-2338.

Lee, B., F.M. Richards, 1971, The interpretation of protein structures: estimation of static accessibility, **J Mol Biol.,** 55, 379-380.

Lieberman, J., E. Song, S. Lee, P. Shankar, 2003, Interfering with Disease: Opportunities and roadblocks to harnessing RNA interferences, **TRENDS in Molecular Medicine.,** 9, 9.

Lindahl, E., B. Hess, D. van der Spoel, 2001, GROMACS 3.0: a package for molecular simulation and trajectory analysis, **J Mol Model.,** 7, 306-317.
Ma, J., K. Ye, D. J. Patel, 2006, Strutural basis for overhang-spesific small interfering RNA recognition by the PAZ domain, **Nature.,** 429, 318-322.

Norberg, J., L. Nilson, 2003, Advances in biomaolecular simulations: methodology, and recent applications, **Quartely Reviews of Biophysics.,** 36, 257-306.

Pande, V., L. Nilson, 2008, Insights into structure, dynamics and hydration of locked nucleic acid (LNA) strand-based duplexes from molecular dynamics simulations, **Nucleic Acids Research.,** 36, 1508-1516.

Reynolds, J.A and Tanford C., 2003, **Nature's Robots: A History of Proteins (Oxford Paperbacks)**, Oxford University Press, USA , 15.

Saenger, W., 1984, **Principle of Nucleic Acid Structure**, Springer-Verlag, New York, 119

Song, J.J., J. Liu, N. H. Tolia, J. Schneiderman, S. K. Smith, R. A. Martienssen, G. J. Hannon, L. J. Tor, 2003, The Crystal Structure of the Argonaute2 PAZ domain reveals an RNA-binding motif in RNAi effector complexes, **Natural structure biology.,** 10, 1026-1032.

Sumner, J.B., 1926, The Isolation and Crystallization of the Enzym Urease, **J. Biol. Chem.,** 69, 435-441.

Van der Spoel, D., E. Lindahl, B. Hess, G. Groenhof, A.E. Mark, H.J.C. Berendsen, 2005, GROMACS: Fast. Flexible, and free, **J Comput Chem.,** 26, 1701-1718.

Van Gusteren, W.F., 1998, Validation of molecular dynamics simulation, **J Chem Phsy.,** 108, 6109-6116

Weiner, P.K., P.A. Kollmann, 1981, AMBER: assisted model building with energy refinement. A general program for modelling molecules and their interactions, **J Comput Chem.,** 2, 287-303.