

## **BAB 5**

### **KESIMPULAN DAN SARAN**

#### **5.1 Kesimpulan Penelitian**

Berdasarkan dari penelitian simulasi dinamika molekul bentuk a po protein *macrophage infectivity potentiator* dari *Legionella pneumophila*, telah diperoleh hasil data sehingga dapat ditarik kesimpulan. Kesimpulan tersebut dipaparkan sebagai berikut:

1. Simulasi dinamika molekul selama 40 ns menghasilkan perhitungan RMSD dengan rata-rata RMSD untuk semua atom protein sebesar 0,39 nm dan untuk atom penyusun tulang belakang sebesar 0,33 nm.
2. Pengaruh potensial *flooding* tidak dapat dilihat dalam simulasi ini karena sistem tidak mencapai kesetimbangan selama 40 ns.
3. Hasil rata-rata nilai perhitungan RMSF untuk semua atom protein memiliki rata-rata sebesar 0,29 nm, sedangkan untuk atom penyusun tulang belakang memiliki rata-rata sebesar 0,16 nm.
4. Residu yang bersifat paling fleksibel berdasarkan penomoran sub bagian pada RMSF adalah F77 (sub bagian 7) dan Q81, V82, I83, Y109, P117, I118 (sub bagian 13).
5. Interaksi ikatan hidrogen Mip yang dapat mempertahankan kestabilan struktur yaitu pada residu T50, Q78, Y55, D66, G57, S67, T68, I83, W86, I101, F126, T87, Q81, L90, Y109 dan R112.

#### **5.2 Saran**

Penelitian ini dapat dilanjutkan dengan:  
Simulasi dinamika molekul protein Mip menggunakan ligan lain.

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