BAB 5
KESIMPULAN DAN SARAN

5.1 Kesimpulan

Berdasarkan hasil penelitian dari simulasi dinamika kompleks FKBP12-*Rapamycin* pada konsentrasi garam fisiologis yang dilakukan selama 400 ns, maka dapat disimpulkan bahwa :

1. Simulasi dinamika kompleks yang dilakukan selama 400 ns menghasilkan nilai rata-rata dari perhitungan RMSD untuk semua atom protein 0,1506 nm dan atom tulang belakang 0,0812 nm.
2. Hasil nilai rata-rata dari perhitungan RMSF untuk semua atom protein 0,1021 nm atom tulang belakang 0,0537 nm.
3. Interaksi ikatan hidrogen yang terbentuk selama waktu simulasi 400 ns yaitu pada residu I56, Y82, D37, E54, Q53.
4. Interaksi ikatan hidrofobik antara residu W59 dengan gugus pipekolil dengan ligan *rapamycin*, stabil dengan jarak rata-rata yang dihasilkan 0,4571 nm

5.2 Saran

Pada penelitian simulasi dinamika kompleks FKBP12-*Rapamycin* pada konsentrasi garam fisiologis dapat dilanjutkan dengan perhitungan energi bebas.

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