

## BAB 5

### KESIMPULAN DAN SARAN

#### 5.1 Kesimpulan

Berdasarkan penelitian pada simulasi dinamika molekul bentuk apo protein FKBP12 (PDB:1FKT) memperoleh hasil data sehingga dapat ditarik kesimpulan. Kesimpulan yang didapatkan adalah sebagai berikut:

1. Simulasi dinamika molekul selama 40 ns menghasilkan rata-rata nilai perhitungan RMSD untuk semua atom protein memiliki rata-rata 0,33 nm, sedangkan untuk atom penyusun tulang belakang protein memiliki rata-rata 0,24 nm.
2. Hasil rata-rata nilai perhitungan RMSF untuk semua atom protein memiliki rata-rata 0,21 nm, sedangkan untuk atom penyusun tulang belakang memiliki rata-rata 0,15 nm.
3. Potensial *flooding* meningkatkan nilai RMSD dan RMSF pada sub bagian 5 dan 6.
4. Residu yang memiliki fleksibilitas tinggi berdasarkan penomoran sub bagian pada RMSF adalah F36 pada sub bagian 5.
5. Interaksi ikatan hidrogen yang hilang setelah pemberian potensial *flooding* adalah Y26 dengan D37.
6. Interaksi ikatan hidrogen yang tetap ada setelah pemberian potensial *flooding* adalah S38 dengan D37, R57 dengan V55.

#### 5.2 Saran

Pada penelitian ini dapat dilanjutkan dengan :  
Simulasi dinamika molekul protein FKBP12 dengan ligan yang lain.

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