ABD24: MHC Class I A*0201- GILGFVFTL-V β 17V α 10.2 TCR complex

Convergence diagnostics of number density

Georgios S.E. Antipas

Molecular Modelling Laboratory, Park Innovaare, CH-5234 Villigen, Switzerland

*Email: gantipas@mmlpi.ch, Tel. +41(0)445862050

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A. Study scope Quantum Immunology ^{1-21} Protein short-range order (SRO) ^{22-38}	B. Methods Molecular dynamics Parameter set: CHARMM22 Water model: TIP3P Solvent padding: 40 Å Periodic boundary conditions: Yes MD Ensemble: Isothermal–isobaric (NPT) Room temperature (RT): 21 °C Physiological temperature (PT): 37 °C Convergence diagnostics Competing Mode Decomposition
C. pMHC-TCR complex details MHC type: A*201 (Homo sapiens) MHC sequence GSHSMRYFFTSVSRPGRGEPFRFIAVGYYDDTQFVRFDSDAASQRMFPAPWIEQEGPEYWDGETRKVKAHSQTHRVDLGTLRGYYNQSEAGSHTVQRMYGCDVGS DWRFLRGYHQYAYDGKDYIALKEDLRSWTAADMAAQTTKHKWEAAHVAEQLRAYLEGTCVEWLRRLRYLENGKETLQRTDAPKTHMTHHAVSDHEATLRCWALSFP AEITLTWQRDGEDQTQDTELVEPTRPAGDGT FQKWA AVVVP SGQE QRYTCHVQHEGLPKPLTLRWEF MHC mutations: None Peptide gene/comments: Homo sapiens Peptide sequence GILGFVFTL TCR type: V β 17V α 10.2 (Homo sapiens) TCR-α sequence MQLLEQSPQFLSIQEGENLTVYCNSSSVFSSSLQWYRQEPGEGPVLLVTVTGGEVKKLKRITFQFGDARKDSSLHITAAQPGDTGLYLCAGAGSQGNLIFGKGTKLSVKPNIQNPDPVAVYQLRDSKSSDKSVCLFTDFDSQTNVSQSKDSDVYITDKTVLDMRSMDFKSNSAVAWSNKSDFACANAFNNSIIPEDTFFPSPENDGGGCKHHHHHH TCR-α mutations: None TCR-β sequence MVDGGITQSPKYLFRKEGQNVTLSCFQNLNHDAMYWYRQDPGQGLRLIYYSQIVNDFQKGDIAEGYSVSREKKESFPLTVTSAQKNPTAFYLCASSRSSYEQYFGPGTRLTVTEDLKNVFPPEVAVFEPSEAEISHTQKATLVCLATGFYPDHVELSWVNGKEVHSGVSTDPQPLKEQPALNDSRYSLSSRLRVSATFWQNPRNHFRQCQVQFYGLSE NDEWTQDRAKPVTTQIVSAEAWGRADQDRGGGCD TCR-β mutations: None

Figure 1. ABD24 supercell number density, ρ , vs. MD time for (a) RT and (d) PT. CMD convergence analysis of ρ vs. MD time for (b) RT and (e) PT. (c) Probability density function of the RT ρ trajectory (Fig.2a), blue bars, and of the RT ρ sample means (sample size of 30), yellow bars. (f) Probability density function of the PT ρ trajectory (Fig.2d), blue bars, and of the PT ρ sample means (sample size of 30), yellow bars. See Table 1 for convergence diagnostics.

Table 1. Convergence diagnostics.

Temperature: RT

Time (ns): 64.5

Type: full

Residual time for full convergence (ns): None

Temperature: PT

Time (ns): 126.3

Type: full

Residual time for full convergence (ns): None

Conflict of interest

The author(s) declare that there is no conflict of interest.

Author contributions

Analysis was based on precursor theoretical modelling related to atomic and mesoscale systems^{1-19,22-67}.

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