ABD6: MHC Class I A*0201-LLFGYPVYV-B7 TCR complex

Convergence diagnostics of number density

Georgios S.E. Antipas*, Nikolaos A. Ntallis

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

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

Keywords: Quantum Immunology, Major Histocompatibility Complex (MHC), peptide (p), T Cell Receptor (TCR), Molecular Dynamics (MD), Competing Mode Decomposition (CMD).

A. Study scope Quantum Immunology ¹⁻¹⁵ Protein short-range order (SRO) ¹⁶⁻³²	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): 25 °C Physiological temperature (PT): 37 °C Convergence diagnostics Competing Mode Decomposition
C. pMHC-TCR complex details MHC type: A*0201 (Homo sapiens) MHC sequence GSHSMRYFFTSVSRPGRGEPFRFIAVGYYDDTQFVRFSDAASQRMFPAPWIEQEGPEYWDGETRKYKAHSQT HRVDLGTLRGYNQSEAGSHTVQRMYGCDVGSQDWRFLRGYHQYAYDGKDYIALKEDLRSWTAADMAAQTTKHK WEAAHVAEQLRAYLEGTCVEWLRRLYLENGKETLQRTDAPKTHMTHHAVSDHEATLRCWALSFPYPAEITLTWQR DGEDQTQDTELVEVTRPAGDGTQKWAADVVPSPGQEQRYTCHVQHEGLPKPLTLRWE MHC mutations: None Peptide gene/comments: TAX protein of human T-lymphotropic virus type 1 Peptide sequence LLFGYPVYV TCR type: B7 (Homo sapiens) TCR-α sequence QQVKQNSPQLSVQEGRISILNCDYTNSMFDYFLWYKKYPAEGPTFLISSIKDKNADGRFTVFLNKSAAHLS LHIVPSQPGDSAVYFCAAMEGAQKLVFGQGTRLTINPNIQNPDPVAVYQLRDSKSSDKSVCLFTDFDSQTNVSQ SKSDSVYITDKTVLDMRSMDFKSNSAVAWSNKSDFACANAFNNSIIPEDTFFPSPSS TCR-α mutations: None TCR-β sequence NAGVTQTPKFQVLKTGQSMTLQCAQDMNHEYMSWYRQDPGMGLRLIHYSVGAGITDQGEVPNGYNVSRSTED FPLRLLSAAPSQTSVYFCASSYPGGGFYEQYFGPGTRLTVTEDLKNVFPPEVAVFEPSEAEISHTQKATLVCL ATGFYPDHVELSWVWNGKEVHSGVSTDPQPLKEQPALNDSRYALSSRLRVSATFWQDPRNHFRQCQVQFYGLSE NDEWTQDRAKPVTQIVSAEAWGRAD TCR-β mutations: None

Figure 1. 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.1a), 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.1d), 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): 119.1

Type: partial

Residual time for full convergence (ns): 60.1

Temperature: PT

Time (ns): 57.9

Type: partial

Residual time for full convergence (ns): 38.0

Conflict of interest

It is declared that there is no conflict of interest.

Author contributions

Analysis was based on precursor theoretical modelling related to atomic and mesoscale systems^{1-12,16-61}.

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