ABE1: MHC Class I A*0201-LLFGYPVYV-A6 TCR complex

Convergence diagnostics of internal energy

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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 ¹⁻⁷ Protein short-range order (SRO) ⁸⁻²⁴	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 GSHSMRYFFTSVSRPGRGEPFIAVG YVDDTQFVRFDSDAASQRM EPAPWIEQEGPEYWDGETR KVKAHSQTHRVDLGLT RGYYNQSEAGSHTVQRM YGCDVGS DWRFLRGYHQYAYDGKDYIALKEDLR SWTAADMAAQTTKHKWEAAHVAEQLRAYLEG TCVEWLRRLYLENGKETLQRTDAPKTHMTHHAVSDHEATLRCWALSFP AEITLTWQRDGEDQTQDTEL VETRPAGDGT FQK WAAVVVPSGQEQR YTCHVQHEGLPKPLTLRWE MHC mutations: None Peptide gene/comments TAX protein of human T-lymphotropic virus type 1 Peptide sequence LLFGYPVYV TCR type: A6 (Homo sapiens) TCR-α sequence KEVEQNSGPLSVPEGAIASLNCTYS DRGSQSFFWYRQYSGKSP ELIMSIYSNGDKEDGRFTAQLNKASQYVSL LIRDSQPS DSATYLC AVTTDSWGLQFGAGTQVVVTPDIQNPDPAVYQLRDSKSSDKSVCLFTDFDSQTNVSQSKDSDVYITDKTVLDM RSMDFKSNSA VAWSNKSDFACANAFNNSIIPEDTFFPSPESS TCR-α mutations: None TCR-β sequence NAGVTQT PKFQVLKTGQSM TLQCAQDMNHEYMSWYRQDPGMGLRLIHYSVGAGITDQGEVPNGYNVSRSTTEDFPLRLLSA APSQTSVYFCASRPGLAGGRPEQYFGPGTRLTVTEDLKNVFPPEVAVFEPSEAEISHTQKATLVCLATGFYPDHVELSWWV NGKEVHSGVSTDPQPLKEQPALNDSRYALSSRLRVSATFWQNPRNHFRQCQVQFYGLSENDEWTQDRAKPVTQIVSAEAWGR AD TCR-β mutations: None

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

Table 1. Convergence diagnostics.

Temperature: RT

Time (ns): 147.8

Type: partial

Residual time for full convergence (ns): 30.4

Temperature: PT

Time (ns): 78.0

Type: full

Residual time for full convergence (ns): None

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 systems¹⁻⁵⁸.

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