ABE23: MHC Class I H-2K^{bm3}- EQYKFYSV-2C 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 ¹⁻²⁰ Protein short-range order (SRO) ²¹⁻³⁷	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): 23 °C Physiological temperature (PT): 37 °C Convergence diagnostics Competing Mode Decomposition
C. pMHC-TCR complex details MHC type: H-2K ^{bm3} (Mus musculus) MHC sequence GPHSLRYFVTAVSRPGLGEPYMEVGYYDDTEFVRFDSDAENPRYEPRARWMEQEGPEYWERETQKAKGNEQS FRVSLRLLGYYNQSAGGSHTIQVISGCEVGSDGRLLRGYQQYAYDGCYIALNEDLKTWTAADMAALITKHK WEQAGEAERLRAYLEGTCVEWLRRLKNGNATLLRTDSPKAHVTHHSRPEDKVTLCWALGFYPADITLTWQL NGEELIQDMELVETRPAGDGTFOKWASVVVPLGKEQYYTCHVYHQGLPEPLTLRWR MHC mutations: None Peptide gene/comments: Mus musculus Peptide sequence EQYKFYSV TCR type: 2C (Mus musculus) TCR-α sequence QSVTQPDARVTVSEGASLQLRCKYSYSATPYLFWYVQYPRQGLQLLLKYYSGDPVVGNGFEAEFSKSNSSF HLRKASVHWSDSAVYFCASGGGTLTYFGAGTRLSVLEDLRNVTTPPKVSLFEPKAEIANKQKATLVCLARGF KTMESGTFITDATVLDMKAMDSKSNGAIAWSNQTSTFCQDIFKETNATYPSSDVPC TCR-α mutations: None TCR-β sequence EAAVTQSPRNKVAVTGGKVTLSNQTNNHNNMYWYRQDTGHGLRLIHYSYGAGSTEKGDIPDGYKASRPSQEN FSLILELATPSQTSVYFCASGGGTLTYFGAGTRLSVLEDLRNVTTPPKVSLFEPKAEIANKQKATLVCLARGF FPDHVELSWVNGKEVHSGVSTDPQAYKESNYSYCLSSRLRVSATFWHNPRNHFRQCQVQFHGLSEEDKWPEGS PKPVTQNI SAEAWGRADC TCR-β mutations: None

Figure 1. ABE23 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 PT E sample means (sample size of 30), yellow bars. See Table 1 for convergence diagnostics.

Table 1. Convergence diagnostics.

Temperature: RT

Time (ns): 97.1

Type: full

Residual time for full convergence (ns): None

Temperature: PT

Time (ns): 19.9

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 systems¹⁻⁶⁶.

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