ABD23: MHC Class I H-2K^{bm3}-EQYKFYSV-2C TCR complex

Convergence diagnostics of number density

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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 ¹⁻¹⁹ Protein short-range order (SRO) ²⁰⁻³⁶	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 QSVTQPDARVTVSEGLQLRCKYSYSATPYLFWYVQYPRQGLQLLLKYSGDPVVQGVNGFEAEFSKSNSSF HLRKASVHWSDSAVYFCVSGFASALTFGSGTKVIVLPYIQNPEPAVYALKDPRSQDSTLCLFTDFDSQINVP KTMESGTFITDATVLDKAMDSKSNGAIAWSNQTSTFCQDIFKETNATYPSSDVPC TCR-α mutations: None TCR-β sequence EAAVTQSPRNKVAVTGGKVTLSNQTNNHNNMYWYRQDTGHGLRLIHYSYGAGSTEKGDIPDGYKASRPSQEN FSLILELATPSQTSVYFCASGGGGTLYFGAGTRLSVLEDLRNVTPPKVSLFEPKAEIANKQKATLVCLARGF FPDHVELSWVNGKEVHSGVSTDPQAYKESNYSYCLSSRLRVSATFWHNPRNHFRQCQVQFHGLSEEDKWPEGS PKPVTQNISAEAWGRADC TCR-β mutations: None

Figure 1. ABD23 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 systems¹⁻⁶⁵.

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