***eLife’s* transparent reporting form**

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* You should state whether an appropriate sample size was computed when the study was being designed
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Our computational analysis of the TCR – CD3 complex is based on 6000 simulation conformations from 120 independent MD simulation trajectories as described in the Results and Methods sections.

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We have generated 120 independent MD trajectories with a length of one microsecond as described in the Results and Methods sections.

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The reported errors have been estimated as the error of the mean of averages obtained for independent subsets of the MD conformations as described in the figure captions.

(For large datasets, or papers with a very large number of statistical tests, you may upload a single table file with tests, Ns, etc., with reference to sections in the manuscript.)

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All 6000 simulation structures on which our data analysis is based are available at the Edmond Open Research Data Repository at: Pandey, P. R. and Weikl, T. R. (2021).

MD simulation structures of the membrane-embedded TCR - CD3 complex. Max Planck Society. https://dx.doi.org/10.17617/3.5m.