were cut off at 10 Å. Smooth particle mesh Ewald was adopted for evaluating long-range electrostatic interactions (Ewald tolerance = $10^{-9}$). The lengths of bonds involving hydrogen atoms were constrained using M-SHAKE[42]. A RESPA integrator (2 fs time-step, long range electrostatics calculated every 6 fs) was used to accumulate 250 ns of simulated time for each system[43]. Trajectories were analysed using VMD[44].

**Data availability.** Atomic co-ordinates and structure factors have been deposited in the Protein Data Bank (PDB) under accession code 5O9H. The data that support the findings of this study are available from the corresponding author upon reasonable request.


29. Caffrey, M. & Cherezov, V. Crystallizing membrane proteins using lipidic mesophases. *Nat. Protocols* **4,** 706–731 (2009).
30. Kabsch, W. XDS. *Acta Crystallogr. D* **66,** 125–132 (2010).
31. Evans, P. R. & Murshudov, G. N. How good are my data and what is the resolution? *Acta Crystallogr. D* **69,** 1204–1214 (2013).
32. Collaborative Computational Project, Number 4. The *CCP*4 suite: programs for protein crystallography. *Acta Crystallogr. D* **50,** 760–763 (1994).
33. Winn, M. D. *et al.* Overview of the CCP4 suite and current developments. *Acta Crystallogr. D* **67,** 235–242 (2011).
34. McCoy, A. J. *et al.* Phaser crystallographic software. *J. Appl. Crystallogr.* **40,** 658–674 (2007).
35. Murshudov, G. N. *et al.* REFMAC5 for the refinement of macromolecular crystal structures. *Acta Crystallogr. D* **67,** 355–367 (2011).
36. Emsley, P., Lohkamp, B., Scott, W. G. & Cowtan, K. Features and development of Coot. *Acta Crystallogr. D* **66,** 486–501 (2010).
37. Adams, P. D. *et al.* PHENIX: a comprehensive Python-based system for macromolecular structure solution. *Acta Crystallogr. D* **66,** 213–221 (2010).
38. Chen, V. B. *et al.* MolProbity: all-atom structure validation for macromolecular crystallography. *Acta Crystallogr. D* **66,** 12–21 (2010).
39. Harder, E. *et al.* OPLS3: a force field providing broad coverage of drug-like small molecules and proteins. *J. Chem. Theory Comput.* **12,** 281–296 (2016).
40. Martyna, G. J., Klein, M. L. & Tuckerman, M. Nosé-Hoover chains: the canonical emsemble via continuous dynamics. *J. Chem. Phys.* **97,** 2635–2643 (1992).
41. Martyna, G. J., Tobias, D. J. & Klein, M. L. Constant pressure molecular dynamics algorithms. *J. Chem. Phys.* **101,** 4177–4189 (1994).
42. Kräutler, V., van Gunsteren, W. F. & Hunenberger, P. H. A fast SHAKE algorithm to solve distance constraint equations for small molecules in molecular dynamics simulations. *J. Comput. Chem.* **22,** 501–508 (2001).
43. Tuckerman, M., Berne, B. J. & Martyna, G. J. Reversible multiple time scale molecular dynamics. *J. Chem. Phys.* **97,** 1990–2001 (1992).
44. Humphrey, W., Dalke, A. & Schulten, K. VMD: visual molecular dynamics. *J. Mol. Graph.* **14,** 33–38, 27–28 (1996).