71 Barrels & corks in a computer - modelling bacterial iron transport systems

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The crystal structures of the outer membrane proteins FhuA and FepA from E. coli have recently been determined (Ferguson et al., Locher et al. and Buchanan et al.). These iron transporters pose an intriguing challenge to our current understanding of the Fe transport mechanism as the beta barrel is occluded by a globular N-terminal domain, the 'cork'. Whether this part of the protein 'unplugs' during transport or undergoes a massive conformational change is unknown.
Molecular dynamics simulations are a useful tool to probe the conformational dynamics of such systems, but they require a complete all-atom model as starting structure. The work presented shows how such a model can be devised using a number of computational techniques to model the protein and its environment accurately enough to reproduce the essential features of the system. First simulation results will also be presented.
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References
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