

Abstract Submitted
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Virtual knotting in proteins and other open curves¹ KEITH ALEXANDER, ALEXANDER TAYLOR, MARK DENNIS, Univ of Bristol — Long filaments naturally knot, from string to long-chain molecules. Knotting in a filament affects its properties, and may be very stable or disappear under slight manipulation. Knotting has been identified in protein backbones for which these mechanical constraints are of fundamental importance to their function [1], although they are open curves in which knots are not mathematically well defined; knotting can only be identified by closing the ends of the chain. We introduce a new method for resolving knotting in open curves using virtual knots [2], a wider class of topological objects that do not use a classical closure, capturing the topological ambiguity of open curves. Having analysed all proteins in the Protein Data Bank by this new scheme, we recover and extend previous knotting results, and identify topological interest in some new cases. The statistics of virtual knots in proteins are compared with those of Hamiltonian subchains on cubic lattices [3], identifying a regime of open curves in which the virtual knotting description is likely to be important [4].

[1] M Jamroz et al, *Nuc Acids Res* 43, D30614 (2014)

[2] L H Kauffman, *Eur J Combin* 20, 66390 (1999)

[3] R C Lua A Y Grosberg, *PLoS Comput Biol* 2, e45 (2006)

[4] K Alexander et al, submitted (2016)

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