MS05-2-5 Racemic crystal structures of A-DNA duplexes
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Abstract
The ease with which racemic mixtures crystallize compared to equivalent chiral systems is a phenomenon with which chemists are highly familiar. However, biological macromolecules such as DNA and proteins are naturally chiral, and thus the limited range of chiral space groups available hampers crystallisation of such molecules. Inspiring work over the past 15 years has shown that racemic mixtures of proteins – made possible by impressive advances in protein chemical synthesis – can indeed improve the success rate of protein crystallisation experiments. More recently, the racemic crystallisation approach was extended to include nucleic acids. Thus, the use of racemic mixtures of nucleic acids may aid in the determination of enantiopure DNA crystal structures. Here, we report findings that suggest that benefits may extend beyond this. We describe two racemic crystal structures of the DNA sequence d(CCCGGG) which we find to fold into A-form DNA. This form differs from the Z-form DNA conformation adopted by the chiral equivalent in the solid state, showing that the use of racemates may also favour the emergence of new conformations. Importantly, the racemic mixture forms interactions in the solid state that differ from the chiral equivalent (including the formation of racemic pseudo-helices), suggesting that the use of racemic DNA mixtures could provide new possibilities towards the design of precise self-assembled nano-materials and nano-structures.

References
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L/D- d(CCCGGG)2 in two racemic crystal forms