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Supporting information for article:

Cryo-neutron crystallographic data collection and preliminary refinement of left-handed Z-DNA d(CGCGCG)

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Table S1 Data collection and refinement statistics.

Z-DNA	
Wavelength	
Resolution range	10.58 - 1.694 (1.754 - 1.694)
Space group	<i>P</i> 21 21 21
Unit cell dimensions	17.8894, 30.768, 43.7051; 90, 90, 90
Total reflections	
Unique reflections	2662 (223)
Multiplicity	
Completeness (%)	90.12 (77.82)
Mean $I/\sigma(I)$	
Wilson B-factor	10.95
R-merge	
R-meas	
R-pim	
CC1/2	
Reflections used in refinement	2655 (221)
Reflections used for R-free	130 (8)
R-work	0.2554 (0.3269)
R-free	0.2824 (0.3702)
Number of non-hydrogen atoms	267
macromolecules	240
solvent	27
Protein residues	0
RMS(bonds)	0.012
RMS(angles)	0.94

Ramachandran favored (%)	0.00
Ramachandran allowed (%)	0.00
Ramachandran outliers (%)	0.00
Rotamer outliers (%)	0.00
Clashscore	10.00
Average B-factor	24.94
macromolecules	22.73
solvent	36.14

Statistics for the highest-resolution shell are shown in parentheses.