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Organic and Bio-organic Chemistry

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Cell Dimensions with Standard Deviations

a(Å)	b(Å)	c(Å)
alpha	beta	gamma

Volume	Mol.Weight	Dm	Dx	Z	Space Group
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Corrected Bond Lengths in Paper <input type="checkbox"/> Yes <input type="checkbox"/> No	Temp(°K)	Mp(°C)	Powder Data <input type="checkbox"/> Yes <input type="checkbox"/> No	Radiation <input type="checkbox"/> X <input type="checkbox"/> N
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Absolute Configuration <input type="checkbox"/> Yes <input type="checkbox"/> No	Colour	Polymorph Indicator	CAS Registry Number
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Drug (indicate, where appropriate, type of drug, activity, etc.)

Chemical Classification (to be assigned by CCDC staff)

Formula (each residue to be formulated separately)

Diagram (conventional chemical structural diagram)

Disorder (specify nature of disorder with reference to atom labels in coord. list)

Remarks (details of constrained refinement, publication history, etc.)