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1,3-Dibutyl-1*H*-purine-2,6(3*H*,7*H*)-dione

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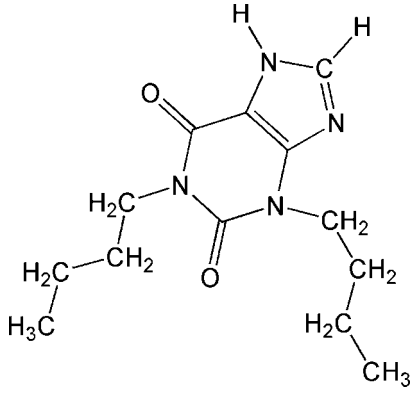
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.002 Å; disorder in main residue; R factor = 0.057; wR factor = 0.147; data-to-parameter ratio = 12.5.

In the crystal structure of the title compound, $C_{13}H_{20}N_4O_2$, the two butyl groups are disordered over two positions, with site-occupancy ratios of 0.56 (2):0.44 (2) and 0.645 (3):0.355 (3). The molecules are linked *via* weak intermolecular N—H···N hydrogen bonds, to form a supramolecular arrangement.

Related literature

For general background, see: Belloni *et al.* (2005); Kahwa *et al.* (1986); Parashar *et al.* (1988); Santos *et al.* (2001); Tynan *et al.* (2005).



Experimental

Crystal data

$C_{13}H_{20}N_4O_2$
M_r = 264.33
Monoclinic, $P2_1/c$
a = 14.2300 (14) Å
b = 9.4120 (8) Å
c = 10.7280 (10) Å
β = 101.290 (4)°
V = 1409.0 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 113 (2) K
0.32 × 0.30 × 0.16 mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.973, T_{max} = 0.986
12057 measured reflections
3070 independent reflections
2515 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.147
S = 1.11
3070 reflections
245 parameters
111 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···N4^{i}	0.99 (2)	1.82 (2)	2.8115 (19)	176.0 (18)

Symmetry code: (i) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CrystalStructure* (Rigaku/MSC, 2005); software used to prepare material for publication: *CrystalStructure*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2387).

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supplementary materials

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1,3-Dibutyl-1*H*-purine-2,6(3*H*,7*H*)-dione

Z.-L. Jing, M. Yu and X. Chen

Comment

In order to establish control over the preparation of crystalline solid materials so that their architecture and properties are predictable (Belloni *et al.*, 2005; Tynan *et al.*, 2005; Parashar *et al.*, 1988), the synthesis of new and designed crystal structures has become a major strand of modern chemistry. Metal complexes based on Schiff bases have attracted much attention because they can be utilized as model compounds of the active centres in various proteins and enzymes (Kahwa *et al.*, 1986; Santos *et al.*, 2001). As part of an investigation of the coordination properties of Shiff bases functioning as ligands, we report the synthesis and crystal structure of the title compound, (I).

In the molecular structure of the compound (I) (Fig. 1), the geometric parameters are normal. In the crystal structurer, the molecules are linked *via* weak intermolecular N–H···N hydrogen bonds (Table 1), to form a supramolecular arrangement, as illustrated in Fig.2.

Experimental

1,3-Dibutyl-1*H*-purine-2,6(3*H*,7H)-dione (1 g) was added to an anhydrous *N*,*N*-dimethylformamide (50 ml), with stirring at 350 K. The resulting colourless solution was filtered and filtrate was allowed to stand in air at room temperature for one month, yielding colourless crystals of (I).

Refinement

The two butyl (C6—C9) and (C10—C13) groups are disordered in two positions with the site-occupancy ratios of 0.564 (1)/0.436 (1) and 0.644 (1)/0.356 (1), respectively. In the disordered group, the *C*(methyl)-*C*(methyl) and *C*(methyl)-*N*(pyrimidine) distances were restrained to 1.54 (1) and 1.48 (1) Å, and the C and N atoms of the minor component were refined isotropically. The N-bound H atom was located in a difference Fourier map and refined freely. C-bound H atoms were included in calculated positions, with C—H = 0.93 (aromatic) or 0.96 Å (methyl), and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C) for aromatic H or 1.5U_{eq}(C) for methyl H atoms.

Figures

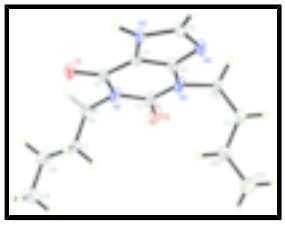

Fig. 1. The structure of the title molecule (I). Displacement ellipsoids are drawn at the 30% probability level. For clarity, only the major disorder components of the atoms are depicted.

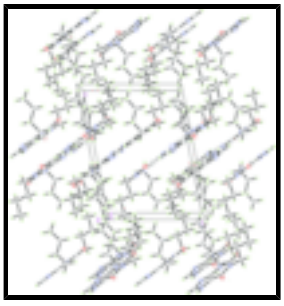

Fig. 2. The crystal packing of (I), viwed down the *b* axis. Hydrogen bonds are indicated by dashed lines.

1,3-Dibutyl-1*H*-purine-2,6(3*H*,7H)-dione

Crystal data

$C_{13}H_{20}N_4O_2$	F_{000} = 568
M_r = 264.33	D_x = 1.246 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71070 Å
Hall symbol: -P 2ybc	Cell parameters from 2683 reflections
a = 14.2300 (14) Å	θ = 2.6–27.9º
b = 9.4120 (8) Å	μ = 0.09 mm^{-1}
c = 10.7280 (10) Å	T = 113 (2) K
β = 101.290 (4)º	Block, colourless
V = 1409.0 (2) Å^3	0.32 × 0.30 × 0.16 mm
Z = 4	

Data collection

Rigaku Saturn diffractometer	3070 independent reflections
Radiation source: rotating anode	2515 reflections with $I > 2\sigma(I)$
Monochromator: confocal	R_{int} = 0.042
T = 113(2) K	θ_{max} = 27.0º
ω scans	θ_{min} = 2.6º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −18→18
T_{min} = 0.973, T_{max} = 0.986	k = −12→11
12057 measured reflections	l = −13→13

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.057	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.147	$w = 1/[\sigma^2(F_o^2) + (0.0761P)^2 + 0.1029P]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 1.11	$(\Delta/\sigma)_{max} < 0.001$
3070 reflections	$\Delta\rho_{max} = 0.21$ e Å^{-3}
245 parameters	$\Delta\rho_{min} = -0.23$ e Å^{-3}
111 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.38973 (8)	0.87003 (12)	0.49767 (10)	0.0374 (3)	
O2	0.25608 (11)	0.47462 (15)	0.28230 (11)	0.0601 (4)	
N1	0.32215 (9)	0.67085 (15)	0.39159 (12)	0.0360 (4)	
N2	0.35377 (10)	0.43656 (14)	0.47432 (12)	0.0367 (4)	
N3	0.48557 (9)	0.66280 (14)	0.70573 (12)	0.0293 (3)	
N4	0.45896 (10)	0.42872 (13)	0.68474 (12)	0.0349 (3)	
C1	0.38066 (11)	0.74015 (17)	0.49472 (13)	0.0308 (4)	
C2	0.30763 (13)	0.52338 (19)	0.37712 (15)	0.0416 (4)	
C3	0.41034 (11)	0.49831 (17)	0.57962 (14)	0.0311 (4)	
C4	0.42479 (11)	0.64183 (16)	0.58947 (14)	0.0289 (4)	
C5	0.50294 (11)	0.53407 (16)	0.75810 (15)	0.0332 (4)	
H5A	0.5425	0.5188	0.8392	0.040*	
C6	0.27299 (11)	0.76074 (19)	0.28581 (15)	0.0395 (4)	
H6A	0.2623	0.7051	0.2093	0.047*	0.56 (2)
H6B	0.3143	0.8383	0.2745	0.047*	0.56 (2)
H6C	0.2623	0.7051	0.2093	0.047*	0.44 (2)
H6D	0.3143	0.8383	0.2745	0.047*	0.44 (2)
C7	0.1760 (4)	0.8211 (10)	0.3046 (8)	0.0415 (16)	0.56 (2)
H7A	0.1304	0.7419	0.3057	0.050*	0.56 (2)
H7B	0.1848	0.8701	0.3878	0.050*	0.56 (2)
C8	0.1341 (4)	0.9254 (11)	0.1991 (8)	0.0501 (18)	0.56 (2)
H8A	0.1291	0.8768	0.1162	0.060*	0.56 (2)
H8B	0.1794	1.0056	0.2008	0.060*	0.56 (2)
C9	0.0357 (4)	0.9851 (14)	0.2079 (7)	0.061 (2)	0.56 (2)
H9A	0.0139	1.0497	0.1364	0.091*	0.56 (2)
H9B	0.0402	1.0371	0.2880	0.091*	0.56 (2)

H9C	−0.0102	0.9069	0.2048	0.091*	0.56 (2)
C10	0.3504 (3)	0.2772 (4)	0.4671 (7)	0.0349 (11)	0.645 (3)
H10A	0.4141	0.2381	0.5049	0.042*	0.645 (3)
H10B	0.3345	0.2474	0.3769	0.042*	0.645 (3)
C11	0.2754 (2)	0.2176 (3)	0.5377 (3)	0.0381 (7)	0.645 (3)
H11A	0.2796	0.1126	0.5384	0.046*	0.645 (3)
H11B	0.2905	0.2506	0.6270	0.046*	0.645 (3)
C12	0.1739 (2)	0.2610 (3)	0.4795 (3)	0.0429 (8)	0.645 (3)
H12A	0.1583	0.2274	0.3904	0.051*	0.645 (3)
H12B	0.1695	0.3659	0.4785	0.051*	0.645 (3)
C13	0.1011 (2)	0.2008 (5)	0.5521 (3)	0.0639 (11)	0.645 (3)
H13A	0.0365	0.2312	0.5110	0.096*	0.645 (3)
H13B	0.1153	0.2355	0.6398	0.096*	0.645 (3)
H13C	0.1044	0.0968	0.5520	0.096*	0.645 (3)
C7'	0.1682 (4)	0.7800 (13)	0.2886 (10)	0.038 (2)	0.44 (2)
H7'A	0.1609	0.8244	0.3699	0.045*	0.44 (2)
H7'B	0.1356	0.6866	0.2814	0.045*	0.44 (2)
C8'	0.1235 (5)	0.8757 (13)	0.1765 (9)	0.045 (2)	0.44 (2)
H8'A	0.1634	0.9619	0.1761	0.054*	0.44 (2)
H8'B	0.1222	0.8243	0.0956	0.054*	0.44 (2)
C9'	0.0225 (5)	0.9189 (16)	0.1858 (9)	0.056 (2)	0.44 (2)
H9'A	−0.0062	0.9736	0.1103	0.085*	0.44 (2)
H9'B	0.0244	0.9773	0.2619	0.085*	0.44 (2)
H9'C	−0.0160	0.8336	0.1914	0.085*	0.44 (2)
C10'	0.3200 (5)	0.2900 (8)	0.4624 (12)	0.032 (2)	0.355 (3)
H10C	0.3723	0.2276	0.5057	0.039*	0.355 (3)
H10D	0.3066	0.2642	0.3712	0.039*	0.355 (3)
C11'	0.2311 (4)	0.2593 (5)	0.5160 (5)	0.0303 (12)	0.355 (3)
H11C	0.1808	0.3296	0.4822	0.036*	0.355 (3)
H11D	0.2465	0.2692	0.6096	0.036*	0.355 (3)
C12'	0.1934 (3)	0.1097 (5)	0.4812 (4)	0.0349 (12)	0.355 (3)
H12C	0.1786	0.1000	0.3875	0.042*	0.355 (3)
H12D	0.2439	0.0398	0.5151	0.042*	0.355 (3)
C13'	0.1040 (3)	0.0768 (6)	0.5334 (5)	0.0423 (14)	0.355 (3)
H13D	0.0857	−0.0226	0.5156	0.063*	0.355 (3)
H13E	0.0516	0.1390	0.4928	0.063*	0.355 (3)
H13F	0.1170	0.0928	0.6254	0.063*	0.355 (3)
H3	0.5081 (14)	0.755 (2)	0.7458 (18)	0.052 (5)*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0494 (7)	0.0245 (7)	0.0324 (6)	−0.0049 (5)	−0.0065 (5)	0.0055 (5)
O2	0.0935 (10)	0.0496 (9)	0.0263 (7)	−0.0352 (7)	−0.0149 (6)	0.0034 (6)
N1	0.0468 (8)	0.0326 (8)	0.0238 (7)	−0.0123 (6)	−0.0046 (6)	0.0061 (6)
N2	0.0573 (9)	0.0245 (8)	0.0243 (7)	−0.0140 (6)	−0.0021 (6)	−0.0006 (5)
N3	0.0398 (7)	0.0183 (7)	0.0254 (7)	−0.0001 (5)	−0.0046 (5)	0.0004 (5)
N4	0.0506 (8)	0.0204 (7)	0.0292 (7)	−0.0015 (6)	−0.0029 (6)	0.0000 (5)

C1	0.0381 (8)	0.0260 (9)	0.0255 (8)	−0.0064 (6)	−0.0005 (6)	0.0031 (6)
C2	0.0604 (11)	0.0355 (10)	0.0248 (8)	−0.0206 (8)	−0.0017 (7)	0.0015 (7)
C3	0.0436 (8)	0.0241 (8)	0.0232 (8)	−0.0053 (6)	0.0006 (6)	−0.0009 (6)
C4	0.0376 (8)	0.0235 (8)	0.0229 (8)	−0.0040 (6)	−0.0007 (6)	−0.0002 (6)
C5	0.0454 (9)	0.0214 (8)	0.0282 (8)	0.0028 (6)	−0.0038 (6)	0.0008 (6)
C6	0.0436 (9)	0.0445 (11)	0.0259 (8)	−0.0127 (7)	−0.0041 (7)	0.0134 (7)
C7	0.038 (2)	0.049 (3)	0.032 (3)	−0.027 (2)	−0.0045 (16)	0.010 (2)
C8	0.039 (2)	0.069 (4)	0.037 (3)	−0.005 (2)	−0.0061 (17)	0.022 (3)
C9	0.045 (2)	0.085 (5)	0.046 (3)	−0.001 (3)	−0.0051 (18)	0.013 (3)
C10	0.052 (3)	0.0205 (17)	0.0289 (17)	−0.0143 (17)	0.000 (2)	−0.0012 (13)
C11	0.0515 (19)	0.0304 (17)	0.0293 (15)	−0.0069 (13)	0.0006 (14)	0.0045 (12)
C12	0.0546 (19)	0.0445 (18)	0.0288 (15)	−0.0035 (15)	0.0063 (14)	0.0047 (12)
C13	0.064 (2)	0.076 (3)	0.054 (2)	−0.0054 (18)	0.0149 (16)	0.0183 (18)
C7'	0.036 (3)	0.049 (4)	0.023 (3)	−0.025 (3)	−0.0071 (18)	0.009 (3)
C8'	0.036 (3)	0.062 (5)	0.033 (3)	−0.012 (3)	−0.002 (2)	0.010 (3)
C9'	0.046 (3)	0.078 (6)	0.041 (3)	−0.005 (3)	−0.001 (2)	0.000 (4)
C10'	0.034 (4)	0.034 (3)	0.028 (3)	−0.006 (3)	0.003 (3)	−0.008 (2)
C11'	0.038 (3)	0.028 (3)	0.022 (3)	−0.001 (2)	−0.001 (2)	−0.001 (2)
C12'	0.041 (2)	0.030 (3)	0.031 (2)	−0.0093 (18)	0.0019 (18)	−0.0001 (19)
C13'	0.041 (2)	0.046 (3)	0.039 (3)	−0.016 (2)	0.006 (2)	0.007 (2)

Geometric parameters (Å, °)

O1—C1	1.2290 (18)	C10—H10A	0.9900
O2—C2	1.2212 (18)	C10—H10B	0.9900
N1—C2	1.407 (2)	C11—C12	1.513 (4)
N1—C1	1.4079 (18)	C11—H11A	0.9900
N1—C6	1.4772 (19)	C11—H11B	0.9900
N2—C3	1.3805 (19)	C12—C13	1.523 (4)
N2—C2	1.385 (2)	C12—H12A	0.9900
N2—C10'	1.458 (7)	C12—H12B	0.9900
N2—C10	1.502 (4)	C13—H13A	0.9800
N3—C5	1.338 (2)	C13—H13B	0.9800
N3—C4	1.3858 (19)	C13—H13C	0.9800
N3—H3	0.99 (2)	C7'—C8'	1.538 (7)
N4—C5	1.3422 (19)	C7'—H7'A	0.9900
N4—C3	1.3689 (19)	C7'—H7'B	0.9900
C1—C4	1.426 (2)	C8'—C9'	1.516 (7)
C3—C4	1.367 (2)	C8'—H8'A	0.9900
C5—H5A	0.9500	C8'—H8'B	0.9900
C6—C7'	1.508 (6)	C9'—H9'A	0.9800
C6—C7	1.542 (6)	C9'—H9'B	0.9800
C6—H6A	0.9600	C9'—H9'C	0.9800
C6—H6B	0.9599	C10'—C11'	1.516 (7)
C6—H6C	0.9600	C10'—H10C	0.9900
C6—H6D	0.9599	C10'—H10D	0.9900
C7—C8	1.528 (6)	C11'—C12'	1.527 (5)
C7—H7A	0.9900	C11'—H11C	0.9900
C7—H7B	0.9900	C11'—H11D	0.9900

C8—C9	1.530 (6)	C12'—C13'	1.519 (5)
C8—H8A	0.9900	C12'—H12C	0.9900
C8—H8B	0.9900	C12'—H12D	0.9900
C9—H9A	0.9800	C13'—H13D	0.9800
C9—H9B	0.9800	C13'—H13E	0.9800
C9—H9C	0.9800	C13'—H13F	0.9800
C10—C11	1.531 (5)		
C2—N1—C1	126.51 (13)	N2—C10—C11	111.0 (4)
C2—N1—C6	116.29 (13)	N2—C10—H10A	109.4
C1—N1—C6	117.17 (13)	C11—C10—H10A	109.4
C3—N2—C2	118.84 (14)	N2—C10—H10B	109.4
C3—N2—C10'	126.8 (5)	C11—C10—H10B	109.4
C2—N2—C10'	113.1 (5)	H10A—C10—H10B	108.0
C3—N2—C10	118.1 (3)	C12—C11—C10	113.5 (3)
C2—N2—C10	123.0 (3)	C12—C11—H11A	108.9
C10'—N2—C10	17.1 (4)	C10—C11—H11A	108.9
C5—N3—C4	106.28 (13)	C12—C11—H11B	108.9
C5—N3—H3	126.3 (11)	C10—C11—H11B	108.9
C4—N3—H3	127.3 (11)	H11A—C11—H11B	107.7
C5—N4—C3	103.42 (12)	C11—C12—C13	112.3 (3)
O1—C1—N1	121.60 (13)	C11—C12—H12A	109.1
O1—C1—C4	126.71 (14)	C13—C12—H12A	109.1
N1—C1—C4	111.69 (13)	C11—C12—H12B	109.1
O2—C2—N2	121.63 (16)	C13—C12—H12B	109.1
O2—C2—N1	120.91 (16)	H12A—C12—H12B	107.9
N2—C2—N1	117.46 (13)	C6—C7'—C8'	108.3 (6)
C4—C3—N4	111.40 (13)	C6—C7'—H7'A	110.0
C4—C3—N2	122.27 (14)	C8'—C7'—H7'A	110.0
N4—C3—N2	126.33 (15)	C6—C7'—H7'B	110.0
C3—C4—N3	105.56 (13)	C8'—C7'—H7'B	110.0
C3—C4—C1	123.19 (13)	H7'A—C7'—H7'B	108.4
N3—C4—C1	131.24 (14)	C9'—C8'—C7'	110.9 (6)
N3—C5—N4	113.34 (13)	C9'—C8'—H8'A	109.5
N3—C5—H5A	123.3	C7'—C8'—H8'A	109.5
N4—C5—H5A	123.3	C9'—C8'—H8'B	109.5
N1—C6—C7'	112.0 (3)	C7'—C8'—H8'B	109.5
N1—C6—C7	114.3 (3)	H8'A—C8'—H8'B	108.0
C7'—C6—C7	16.1 (4)	C8'—C9'—H9'A	109.5
N1—C6—H6A	108.4	C8'—C9'—H9'B	109.5
C7'—C6—H6A	95.2	H9'A—C9'—H9'B	109.5
C7—C6—H6A	108.5	C8'—C9'—H9'C	109.5
N1—C6—H6B	108.8	H9'A—C9'—H9'C	109.5
C7'—C6—H6B	123.0	H9'B—C9'—H9'C	109.5
C7—C6—H6B	108.9	N2—C10'—C11'	115.6 (6)
H6A—C6—H6B	107.7	N2—C10'—H10C	108.4
N1—C6—H6C	108.4	C11'—C10'—H10C	108.4
C7'—C6—H6C	95.2	N2—C10'—H10D	108.4
C7—C6—H6C	108.5	C11'—C10'—H10D	108.4
H6A—C6—H6C	0.0	H10C—C10'—H10D	107.4

H6B—C6—H6C	107.7	C10'—C11'—C12'	111.3 (5)
N1—C6—H6D	108.8	C10'—C11'—H11C	109.4
C7'—C6—H6D	123.0	C12'—C11'—H11C	109.4
C7—C6—H6D	108.9	C10'—C11'—H11D	109.4
H6A—C6—H6D	107.7	C12'—C11'—H11D	109.4
H6B—C6—H6D	0.0	H11C—C11'—H11D	108.0
H6C—C6—H6D	107.7	C13'—C12'—C11'	112.2 (4)
C8—C7—C6	111.6 (5)	C13'—C12'—H12C	109.2
C8—C7—H7A	109.3	C11'—C12'—H12C	109.2
C6—C7—H7A	109.3	C13'—C12'—H12D	109.2
C8—C7—H7B	109.3	C11'—C12'—H12D	109.2
C6—C7—H7B	109.3	H12C—C12'—H12D	107.9
H7A—C7—H7B	108.0	C12'—C13'—H13D	109.5
C7—C8—C9	114.8 (5)	C12'—C13'—H13E	109.5
C7—C8—H8A	108.6	H13D—C13'—H13E	109.5
C9—C8—H8A	108.6	C12'—C13'—H13F	109.5
C7—C8—H8B	108.6	H13D—C13'—H13F	109.5
C9—C8—H8B	108.6	H13E—C13'—H13F	109.5
H8A—C8—H8B	107.5		
C2—N1—C1—O1	178.94 (15)	C5—N3—C4—C1	177.99 (16)
C6—N1—C1—O1	0.8 (2)	O1—C1—C4—C3	179.40 (16)
C2—N1—C1—C4	−1.2 (2)	N1—C1—C4—C3	−0.5 (2)
C6—N1—C1—C4	−179.29 (13)	O1—C1—C4—N3	1.1 (3)
C3—N2—C2—O2	−179.37 (16)	N1—C1—C4—N3	−178.77 (15)
C10'—N2—C2—O2	−11.1 (4)	C4—N3—C5—N4	0.62 (18)
C10—N2—C2—O2	4.7 (3)	C3—N4—C5—N3	−0.42 (18)
C3—N2—C2—N1	0.5 (2)	C2—N1—C6—C7'	78.2 (6)
C10'—N2—C2—N1	168.7 (4)	C1—N1—C6—C7'	−103.5 (6)
C10—N2—C2—N1	−175.4 (3)	C2—N1—C6—C7	95.6 (4)
C1—N1—C2—O2	−178.94 (16)	C1—N1—C6—C7	−86.1 (4)
C6—N1—C2—O2	−0.8 (2)	N1—C6—C7—C8	173.9 (4)
C1—N1—C2—N2	1.2 (2)	C7'—C6—C7—C8	−101 (2)
C6—N1—C2—N2	179.30 (14)	C6—C7—C8—C9	177.5 (5)
C5—N4—C3—C4	0.05 (18)	C3—N2—C10—C11	85.2 (4)
C5—N4—C3—N2	179.53 (15)	C2—N2—C10—C11	−98.8 (4)
C2—N2—C3—C4	−2.1 (2)	C10'—N2—C10—C11	−40 (2)
C10'—N2—C3—C4	−168.5 (4)	N2—C10—C11—C12	64.2 (5)
C10—N2—C3—C4	174.0 (3)	C10—C11—C12—C13	−179.7 (3)
C2—N2—C3—N4	178.47 (15)	N1—C6—C7'—C8'	179.4 (4)
C10'—N2—C3—N4	12.0 (5)	C7—C6—C7'—C8'	77.8 (19)
C10—N2—C3—N4	−5.4 (3)	C6—C7'—C8'—C9'	−170.8 (6)
N4—C3—C4—N3	0.31 (18)	C3—N2—C10'—C11'	82.6 (8)
N2—C3—C4—N3	−179.20 (14)	C2—N2—C10'—C11'	−84.5 (9)
N4—C3—C4—C1	−178.37 (14)	C10—N2—C10'—C11'	147 (3)
N2—C3—C4—C1	2.1 (2)	N2—C10'—C11'—C12'	171.5 (7)
C5—N3—C4—C3	−0.54 (17)	C10'—C11'—C12'—C13'	−179.7 (6)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···N4^{i}	0.99 (2)	1.82 (2)	2.8115 (19)	176.0 (18)

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+3/2.

Fig. 1

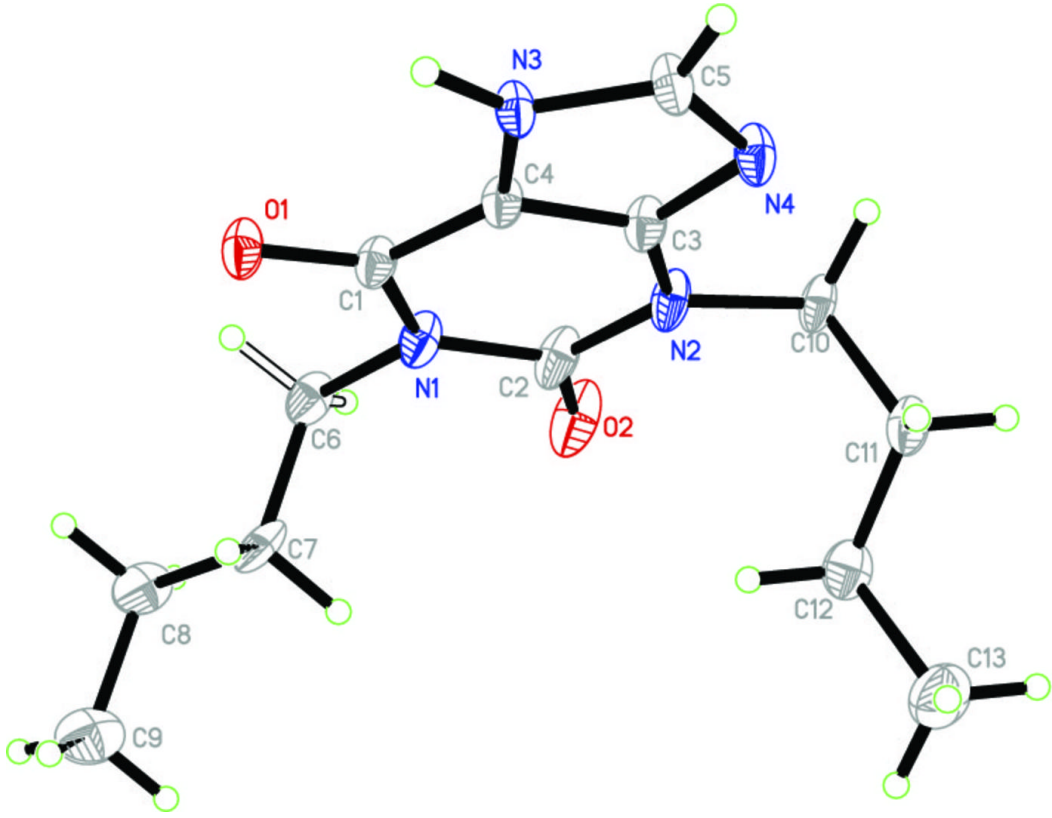

Fig. 2