

1-[(Cyclopropylmethoxy)methyl]-5-ethyl-6-(4-methylbenzyl)-1,2,3,4-tetrahydropyrimidine-2,4-dione

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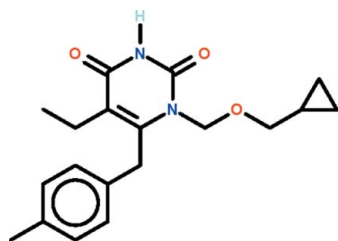
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; disorder in main residue; R factor = 0.061; wR factor = 0.155; data-to-parameter ratio = 17.3.

The pyrimidine ring in the title compound, $\text{C}_{19}\text{H}_{24}\text{N}_2\text{O}_3$, is nearly planar (r.m.s. deviation = 0.008 Å); the C atom at the 5-position deviates by 0.054 (3) Å from the mean plane and the C atom at the 6-position by 0.006 (3) Å in the opposite direction. The benzene ring is approximately perpendicular to the pyrimidine ring [dihedral angle = 83.90 (10)°]. The amino group is hydrogen-bond donor to the exocyclic O atom at the 2-position of an adjacent molecule, the hydrogen bond generating an inversion dimer. The cyclopropyl ring is disordered over two sets of sites with the major component having 71.5 (4)% occupancy.

Related literature

For the synthesis, see: El-Brollosy *et al.* (2009).



Experimental

Crystal data

$\text{C}_{19}\text{H}_{24}\text{N}_2\text{O}_3$
 $M_r = 328.40$
Monoclinic, $C2/c$
 $a = 15.6080$ (13) Å
 $b = 8.1330$ (6) Å
 $c = 27.496$ (2) Å
 $\beta = 93.397$ (7)°

$V = 3484.2$ (5) Å³
 $Z = 8$
Mo $K\alpha$ radiation
 $\mu = 0.09$ mm⁻¹
 $T = 100$ K
0.25 × 0.20 × 0.15 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
 $T_{\min} = 0.979$, $T_{\max} = 0.987$

7060 measured reflections
4006 independent reflections
2446 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.044$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.061$
 $wR(F^2) = 0.155$
 $S = 1.06$
4006 reflections
232 parameters
20 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.22$ e Å⁻³
 $\Delta\rho_{\min} = -0.26$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1}\cdots\text{O1}^i$	0.89 (1)	1.93 (1)	2.816 (2)	178 (2)

Symmetry code: (i) $-x + 1, -y + 1, -z + 1$.

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5423).

References

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supplementary materials

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1-[(Cyclopropylmethoxy)methyl]-5-ethyl-6-(4-methylbenzyl)-1,2,3,4-tetrahydropyrimidine-2,4-dione

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Comment

The compound (Scheme I) was synthesized for an evaluation of its anti-viral activity against HIV-1 (El-Brollosy *et al.*, 2009). The pyrimidine ring is nearly planar; the C atom at the 5-position deviates by 0.054 (3) Å from the mean plane and the C atom at the 6-position by 0.006 (3) Å in the opposite direction (Fig. 1). The amino group is hydrogen-bond donor to the exocyclic O atom at the 2-position, the hydrogen bond generating a centrosymmetric dimer (Table 1, Fig. 2).

Experimental

The compound (Scheme I) was synthesized by using a reported method (El-Brollosy *et al.*, 2009), and was recrystallized from ethanol.

Refinement

Carbon-bound H-atoms were placed in calculated positions [C–H 0.95 to 0.98 Å, $U_{\text{iso}}(\text{H})$ 1.2 to 1.5 $U_{\text{eq}}(\text{C})$] and were included in the refinement in the riding model approximation.

The amino H-atom was located in a difference Fourier map, and was refined with a distance restraint of N–H 0.88±0.01 Å; its temperature factor was refined.

The cyclopropyl ring is disordered over two positions. The pair of C_{methylene}–C_{cyclopropyl} bond distances were restrained to within 0.01±0.01 Å of each other, as were the bond distances of the ring itself. The temperature factors of the primed were set to those of the unprimed ones, and the anisotropic temperature factors were restrained to be nearly isotropic.

Figures

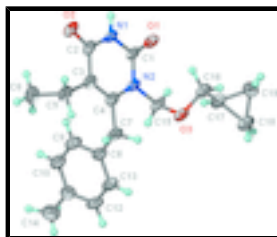


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of C₁₉H₂₄N₂O₃ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius. The disorder is not shown.

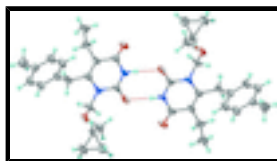


Fig. 2. Dimeric hydrogen-bonded structure.

1-[(Cyclopropylmethoxy)methyl]-5-ethyl-6-(4-methylbenzyl)-1,2,3,4-tetrahydropyrimidine-2,4-dione

Crystal data

$C_{19}H_{24}N_2O_3$	$F(000) = 1408$
$M_r = 328.40$	$D_x = 1.252 \text{ Mg m}^{-3}$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: $-C 2yc$	Cell parameters from 1703 reflections
$a = 15.6080 (13) \text{ \AA}$	$\theta = 2.6\text{--}27.5^\circ$
$b = 8.1330 (6) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$c = 27.496 (2) \text{ \AA}$	$T = 100 \text{ K}$
$\beta = 93.397 (7)^\circ$	Irregular, colorless
$V = 3484.2 (5) \text{ \AA}^3$	$0.25 \times 0.20 \times 0.15 \text{ mm}$
$Z = 8$	

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector	4006 independent reflections
Radiation source: SuperNova (Mo) X-ray Source	2446 reflections with $I > 2\sigma(I)$
Mirror	$R_{\text{int}} = 0.044$
Detector resolution: $10.4041 \text{ pixels mm}^{-1}$	$\theta_{\text{max}} = 27.6^\circ$, $\theta_{\text{min}} = 2.6^\circ$
ω scan	$h = -20 \rightarrow 19$
Absorption correction: multi-scan (<i>CrysAlis PRO</i> ; Agilent, 2010)	$k = -7 \rightarrow 10$
$T_{\text{min}} = 0.979$, $T_{\text{max}} = 0.987$	$l = -35 \rightarrow 21$
7060 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.061$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.155$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.06$	$w = 1/[\sigma^2(F_o^2) + (0.0471P)^2 + 1.5059P]$
4006 reflections	where $P = (F_o^2 + 2F_c^2)/3$
232 parameters	$(\Delta/\sigma)_{\text{max}} = 0.001$
20 restraints	$\Delta\rho_{\text{max}} = 0.22 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.26 \text{ e \AA}^{-3}$

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
O1	0.50675 (10)	0.53293 (18)	0.43772 (5)	0.0306 (4)	

O2	0.72573 (10)	0.51944 (19)	0.55353 (6)	0.0337 (4)	
O3	0.61688 (10)	0.75562 (18)	0.34641 (5)	0.0322 (4)	
N1	0.61833 (12)	0.5257 (2)	0.49464 (7)	0.0252 (4)	
H1	0.5798 (12)	0.508 (3)	0.5165 (7)	0.036 (7)*	
N2	0.64326 (12)	0.5688 (2)	0.41308 (6)	0.0251 (4)	
C1	0.58460 (15)	0.5419 (3)	0.44798 (8)	0.0256 (5)	
C2	0.70469 (15)	0.5330 (2)	0.51006 (8)	0.0260 (5)	
C3	0.76385 (15)	0.5573 (3)	0.47165 (8)	0.0261 (5)	
C4	0.73229 (15)	0.5764 (2)	0.42504 (8)	0.0253 (5)	
C5	0.85735 (15)	0.5580 (3)	0.48899 (9)	0.0316 (6)	
H5A	0.8648	0.6277	0.5184	0.038*	
H5B	0.8913	0.6074	0.4634	0.038*	
C6	0.89235 (16)	0.3854 (3)	0.50097 (10)	0.0394 (6)	
H6A	0.9522	0.3936	0.5136	0.059*	
H6B	0.8891	0.3180	0.4714	0.059*	
H6C	0.8580	0.3344	0.5256	0.059*	
C7	0.78826 (15)	0.6035 (3)	0.38279 (8)	0.0306 (6)	
H7A	0.8437	0.6504	0.3954	0.037*	
H7B	0.7603	0.6858	0.3606	0.037*	
C8	0.80601 (14)	0.4493 (3)	0.35365 (8)	0.0286 (5)	
C9	0.80732 (16)	0.2935 (3)	0.37445 (9)	0.0354 (6)	
H9	0.7922	0.2810	0.4072	0.043*	
C10	0.83032 (16)	0.1554 (3)	0.34834 (8)	0.0354 (6)	
H10	0.8311	0.0506	0.3636	0.042*	
C11	0.85223 (15)	0.1686 (3)	0.30026 (8)	0.0331 (6)	
C12	0.84815 (15)	0.3240 (3)	0.27877 (9)	0.0369 (6)	
H12	0.8607	0.3357	0.2456	0.044*	
C13	0.82606 (15)	0.4618 (3)	0.30501 (8)	0.0340 (6)	
H13	0.8246	0.5664	0.2896	0.041*	
C14	0.87809 (17)	0.0183 (3)	0.27244 (9)	0.0457 (7)	
H14A	0.9128	0.0518	0.2456	0.069*	
H14B	0.8265	-0.0390	0.2593	0.069*	
H14C	0.9117	-0.0554	0.2944	0.069*	
C15	0.60855 (15)	0.5928 (3)	0.36212 (8)	0.0285 (5)	
H15A	0.6393	0.5192	0.3404	0.034*	
H15B	0.5471	0.5617	0.3597	0.034*	
C16	0.55665 (16)	0.8680 (3)	0.36619 (9)	0.0326 (6)	
H16A	0.5479	0.8404	0.4006	0.039*	0.715 (4)
H16B	0.5006	0.8618	0.3474	0.039*	0.715 (4)
H16C	0.5778	0.8995	0.3995	0.039*	0.285 (4)
H16D	0.5009	0.8113	0.3686	0.039*	0.285 (4)
C17	0.5939 (2)	1.0366 (4)	0.36259 (12)	0.0311 (8)	0.715 (4)
H17	0.6480	1.0583	0.3829	0.037*	0.715 (4)
C18	0.5821 (3)	1.1319 (4)	0.31577 (14)	0.0401 (9)	0.715 (4)
H18A	0.6284	1.2083	0.3074	0.048*	0.715 (4)
H18B	0.5518	1.0771	0.2876	0.048*	0.715 (4)
C19	0.5321 (8)	1.1730 (14)	0.3578 (5)	0.0357 (18)	0.715 (4)
H19A	0.4703	1.1451	0.3558	0.043*	0.715 (4)
H19B	0.5467	1.2760	0.3756	0.043*	0.715 (4)

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C17'	0.5430 (5)	1.0209 (9)	0.3360 (3)	0.0311 (8)	0.285
H17'	0.5189	1.0059	0.3018	0.037*	0.285 (4)
C18'	0.6114 (7)	1.1436 (12)	0.3439 (4)	0.0401 (9)	0.285
H18C	0.6306	1.2021	0.3149	0.048*	0.285 (4)
H18D	0.6579	1.1186	0.3688	0.048*	0.285 (4)
C19'	0.521 (2)	1.192 (4)	0.3624 (15)	0.0357 (18)	0.285
H19C	0.4865	1.2742	0.3436	0.043*	0.285 (4)
H19D	0.5140	1.1902	0.3979	0.043*	0.285 (4)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0354 (10)	0.0381 (9)	0.0179 (8)	-0.0015 (7)	-0.0004 (7)	0.0037 (7)
O2	0.0468 (10)	0.0358 (9)	0.0176 (9)	-0.0012 (8)	-0.0050 (7)	0.0035 (7)
O3	0.0479 (10)	0.0299 (8)	0.0192 (9)	0.0014 (8)	0.0055 (7)	0.0056 (7)
N1	0.0359 (11)	0.0256 (10)	0.0140 (10)	-0.0014 (9)	0.0009 (8)	0.0030 (8)
N2	0.0356 (11)	0.0265 (9)	0.0131 (9)	-0.0029 (8)	0.0007 (8)	0.0014 (7)
C1	0.0378 (14)	0.0231 (11)	0.0158 (11)	-0.0015 (10)	0.0010 (10)	0.0027 (9)
C2	0.0398 (14)	0.0184 (10)	0.0191 (12)	0.0003 (10)	-0.0039 (10)	-0.0001 (9)
C3	0.0359 (13)	0.0212 (11)	0.0210 (12)	-0.0011 (10)	-0.0005 (10)	0.0005 (9)
C4	0.0352 (13)	0.0181 (10)	0.0226 (12)	-0.0026 (10)	0.0009 (10)	0.0005 (9)
C5	0.0388 (14)	0.0276 (12)	0.0278 (13)	-0.0026 (11)	-0.0029 (10)	0.0041 (10)
C6	0.0416 (15)	0.0349 (14)	0.0408 (16)	0.0035 (12)	-0.0052 (12)	0.0027 (11)
C7	0.0381 (14)	0.0317 (12)	0.0221 (13)	-0.0057 (11)	0.0034 (10)	0.0044 (10)
C8	0.0297 (12)	0.0378 (13)	0.0183 (12)	-0.0035 (10)	0.0008 (9)	-0.0004 (10)
C9	0.0492 (16)	0.0383 (14)	0.0193 (13)	0.0005 (12)	0.0066 (11)	-0.0012 (10)
C10	0.0508 (15)	0.0362 (13)	0.0191 (13)	0.0040 (12)	0.0018 (11)	-0.0009 (10)
C11	0.0303 (13)	0.0510 (15)	0.0177 (12)	0.0049 (11)	-0.0034 (9)	-0.0066 (11)
C12	0.0370 (14)	0.0591 (17)	0.0148 (12)	-0.0020 (12)	0.0027 (10)	0.0015 (11)
C13	0.0366 (13)	0.0446 (14)	0.0205 (13)	-0.0051 (12)	-0.0001 (10)	0.0044 (11)
C14	0.0458 (16)	0.0653 (18)	0.0256 (14)	0.0110 (14)	-0.0011 (12)	-0.0125 (13)
C15	0.0421 (14)	0.0308 (12)	0.0124 (11)	-0.0009 (11)	-0.0007 (10)	0.0016 (9)
C16	0.0436 (15)	0.0329 (13)	0.0211 (13)	0.0016 (11)	0.0018 (10)	0.0042 (10)
C17	0.0378 (18)	0.0338 (17)	0.0212 (17)	-0.0049 (15)	-0.0034 (12)	0.0026 (14)
C18	0.058 (2)	0.0379 (18)	0.024 (2)	0.0008 (18)	0.0071 (16)	0.0057 (18)
C19	0.045 (4)	0.025 (3)	0.038 (3)	0.006 (2)	0.009 (2)	-0.004 (2)
C17'	0.0378 (18)	0.0338 (17)	0.0212 (17)	-0.0049 (15)	-0.0034 (12)	0.0026 (14)
C18'	0.058 (2)	0.0379 (18)	0.024 (2)	0.0008 (18)	0.0071 (16)	0.0057 (18)
C19'	0.045 (4)	0.025 (3)	0.038 (3)	0.006 (2)	0.009 (2)	-0.004 (2)

Geometric parameters (\AA , $^\circ$)

O1—C1	1.233 (3)	C12—C13	1.387 (3)
O2—C2	1.226 (2)	C12—H12	0.9500
O3—C15	1.401 (3)	C13—H13	0.9500
O3—C16	1.440 (3)	C14—H14A	0.9800
N1—C1	1.364 (3)	C14—H14B	0.9800
N1—C2	1.390 (3)	C14—H14C	0.9800
N1—H1	0.887 (10)	C15—H15A	0.9900

N2—C1	1.382 (3)	C15—H15B	0.9900
N2—C4	1.410 (3)	C16—C17	1.495 (4)
N2—C15	1.485 (3)	C16—C17'	1.503 (7)
C2—C3	1.457 (3)	C16—H16A	0.9900
C3—C4	1.354 (3)	C16—H16B	0.9900
C3—C5	1.508 (3)	C16—H16C	0.9900
C4—C7	1.511 (3)	C16—H16D	0.9900
C5—C6	1.535 (3)	C17—C19	1.471 (12)
C5—H5A	0.9900	C17—C18	1.505 (5)
C5—H5B	0.9900	C17—H17	1.0000
C6—H6A	0.9800	C18—C19	1.472 (12)
C6—H6B	0.9800	C18—H18A	0.9900
C6—H6C	0.9800	C18—H18B	0.9900
C7—C8	1.523 (3)	C19—H19A	0.9900
C7—H7A	0.9900	C19—H19B	0.9900
C7—H7B	0.9900	C17'—C18'	1.468 (14)
C8—C9	1.390 (3)	C17'—C19'	1.61 (3)
C8—C13	1.395 (3)	C17'—H17'	1.0000
C9—C10	1.391 (3)	C18'—C19'	1.57 (3)
C9—H9	0.9500	C18'—H18C	0.9900
C10—C11	1.389 (3)	C18'—H18D	0.9900
C10—H10	0.9500	C19'—H19C	0.9900
C11—C12	1.395 (3)	C19'—H19D	0.9900
C11—C14	1.509 (3)		
C15—O3—C16	114.11 (17)	H14A—C14—H14C	109.5
C1—N1—C2	126.6 (2)	H14B—C14—H14C	109.5
C1—N1—H1	114.4 (16)	O3—C15—N2	112.32 (17)
C2—N1—H1	119.0 (16)	O3—C15—H15A	109.1
C1—N2—C4	121.93 (18)	N2—C15—H15A	109.1
C1—N2—C15	117.14 (18)	O3—C15—H15B	109.1
C4—N2—C15	120.92 (18)	N2—C15—H15B	109.1
O1—C1—N1	122.0 (2)	H15A—C15—H15B	107.9
O1—C1—N2	122.3 (2)	O3—C16—C17	107.0 (2)
N1—C1—N2	115.7 (2)	O3—C16—C17'	113.0 (4)
O2—C2—N1	119.5 (2)	O3—C16—H16A	110.3
O2—C2—C3	125.1 (2)	C17—C16—H16A	110.3
N1—C2—C3	115.44 (19)	C17'—C16—H16A	133.8
C4—C3—C2	119.4 (2)	O3—C16—H16B	110.3
C4—C3—C5	126.1 (2)	C17—C16—H16B	110.3
C2—C3—C5	114.5 (2)	H16A—C16—H16B	108.6
C3—C4—N2	120.9 (2)	O3—C16—H16C	109.0
C3—C4—C7	123.4 (2)	C17—C16—H16C	73.4
N2—C4—C7	115.69 (19)	C17'—C16—H16C	109.0
C3—C5—C6	112.95 (19)	O3—C16—H16D	109.0
C3—C5—H5A	109.0	C17'—C16—H16D	109.0
C6—C5—H5A	109.0	H16C—C16—H16D	107.8
C3—C5—H5B	109.0	C19—C17—C16	116.2 (5)
C6—C5—H5B	109.0	C19—C17—C18	59.3 (6)
H5A—C5—H5B	107.8	C16—C17—C18	120.0 (3)

supplementary materials

C5—C6—H6A	109.5	C19—C17—H17	116.3
C5—C6—H6B	109.5	C16—C17—H17	116.3
H6A—C6—H6B	109.5	C18—C17—H17	116.3
C5—C6—H6C	109.5	C19—C18—C17	59.2 (6)
H6A—C6—H6C	109.5	C19—C18—H18A	117.8
H6B—C6—H6C	109.5	C17—C18—H18A	117.8
C4—C7—C8	114.55 (18)	C19—C18—H18B	117.8
C4—C7—H7A	108.6	C17—C18—H18B	117.8
C8—C7—H7A	108.6	H18A—C18—H18B	115.0
C4—C7—H7B	108.6	C18—C19—C17	61.5 (4)
C8—C7—H7B	108.6	C18—C19—H19A	117.6
H7A—C7—H7B	107.6	C17—C19—H19A	117.6
C9—C8—C13	117.5 (2)	C18—C19—H19B	117.6
C9—C8—C7	122.2 (2)	C17—C19—H19B	117.6
C13—C8—C7	120.2 (2)	H19A—C19—H19B	114.7
C8—C9—C10	121.4 (2)	C18'—C17'—C16	113.8 (7)
C8—C9—H9	119.3	C18'—C17'—C19'	61.3 (12)
C10—C9—H9	119.3	C16—C17'—C19'	119.4 (16)
C11—C10—C9	120.9 (2)	C18'—C17'—H17'	116.8
C11—C10—H10	119.5	C16—C17'—H17'	116.8
C9—C10—H10	119.5	C19'—C17'—H17'	116.8
C10—C11—C12	117.7 (2)	C17'—C18'—C19'	63.9 (12)
C10—C11—C14	120.5 (2)	C17'—C18'—H18C	117.4
C12—C11—C14	121.7 (2)	C19'—C18'—H18C	117.4
C13—C12—C11	121.2 (2)	C17'—C18'—H18D	117.4
C13—C12—H12	119.4	C19'—C18'—H18D	117.4
C11—C12—H12	119.4	H18C—C18'—H18D	114.4
C12—C13—C8	121.1 (2)	C18'—C19'—C17'	54.9 (12)
C12—C13—H13	119.5	C18'—C19'—H19C	118.3
C8—C13—H13	119.5	C17'—C19'—H19C	118.3
C11—C14—H14A	109.5	C18'—C19'—H19D	118.3
C11—C14—H14B	109.5	C17'—C19'—H19D	118.3
H14A—C14—H14B	109.5	H19C—C19'—H19D	115.5
C11—C14—H14C	109.5		
C2—N1—C1—O1	179.7 (2)	C7—C8—C9—C10	-174.8 (2)
C2—N1—C1—N2	-0.2 (3)	C8—C9—C10—C11	-0.5 (4)
C4—N2—C1—O1	-178.97 (19)	C9—C10—C11—C12	-1.6 (4)
C15—N2—C1—O1	2.1 (3)	C9—C10—C11—C14	179.3 (2)
C4—N2—C1—N1	0.9 (3)	C10—C11—C12—C13	2.3 (4)
C15—N2—C1—N1	-177.95 (17)	C14—C11—C12—C13	-178.6 (2)
C1—N1—C2—O2	178.59 (19)	C11—C12—C13—C8	-0.9 (4)
C1—N1—C2—C3	-1.3 (3)	C9—C8—C13—C12	-1.3 (3)
O2—C2—C3—C4	-177.7 (2)	C7—C8—C13—C12	175.6 (2)
N1—C2—C3—C4	2.2 (3)	C16—O3—C15—N2	-75.0 (2)
O2—C2—C3—C5	2.4 (3)	C1—N2—C15—O3	109.0 (2)
N1—C2—C3—C5	-177.65 (17)	C4—N2—C15—O3	-69.9 (2)
C2—C3—C4—N2	-1.7 (3)	C15—O3—C16—C17	158.4 (2)
C5—C3—C4—N2	178.21 (19)	C15—O3—C16—C17'	-158.1 (4)
C2—C3—C4—C7	179.5 (2)	O3—C16—C17—C19	151.7 (6)

C5—C3—C4—C7	-0.7 (3)	C17'—C16—C17—C19	45.9 (8)
C1—N2—C4—C3	0.0 (3)	O3—C16—C17—C18	83.6 (3)
C15—N2—C4—C3	178.87 (18)	C17'—C16—C17—C18	-22.2 (5)
C1—N2—C4—C7	178.97 (19)	C16—C17—C18—C19	104.5 (6)
C15—N2—C4—C7	-2.2 (3)	C16—C17—C19—C18	-110.9 (4)
C4—C3—C5—C6	-104.2 (2)	O3—C16—C17'—C18'	-79.3 (7)
C2—C3—C5—C6	75.6 (3)	C17—C16—C17'—C18'	10.5 (5)
C3—C4—C7—C8	98.1 (2)	O3—C16—C17'—C19'	-148.5 (14)
N2—C4—C7—C8	-80.8 (2)	C17—C16—C17'—C19'	-58.7 (15)
C4—C7—C8—C9	-28.4 (3)	C16—C17'—C18'—C19'	-111.8 (18)
C4—C7—C8—C13	154.9 (2)	C16—C17'—C19'—C18'	102.6 (12)
C13—C8—C9—C10	1.9 (4)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N1—H1 \cdots O1 ⁱ	0.89 (1)	1.93 (1)	2.816 (2)	178 (2)

Symmetry codes: (i) $-x+1, -y+1, -z+1$.

Fig. 1

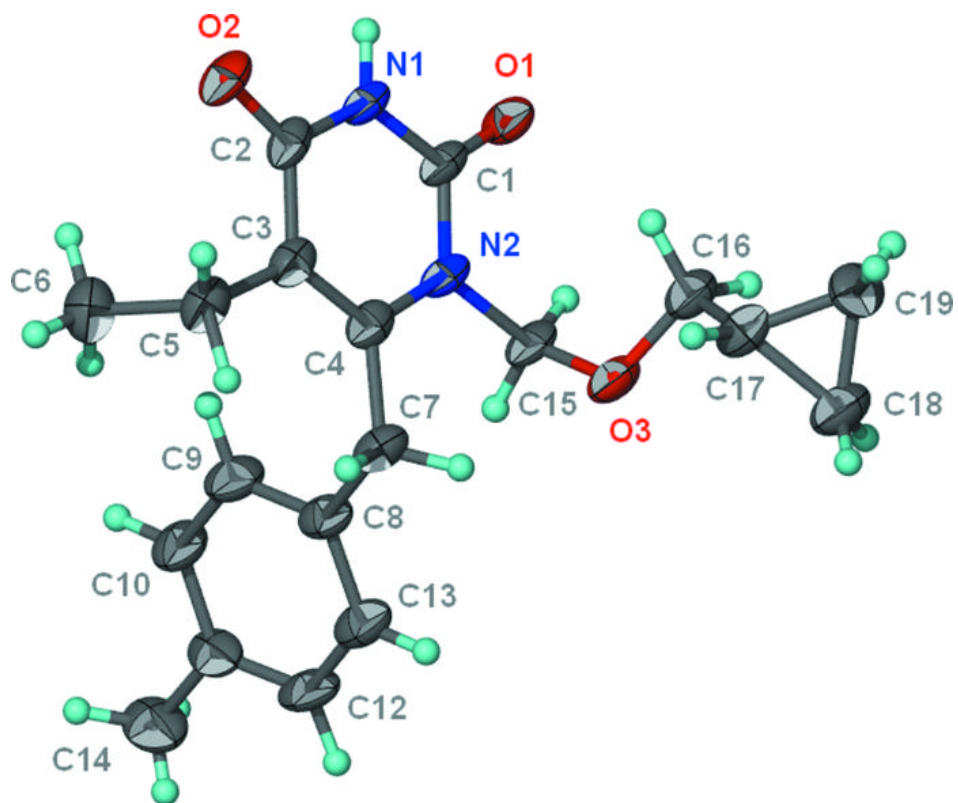


Fig. 2

