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6-[(4-Bromophenyl)iminomethyl]-1,3-dimethyl-7-(2-methylpropenyl)-1,2,3,4-tetrahydro-7*H*-pyrrolo[2,3-*d*]pyrimidine-2,4-dione

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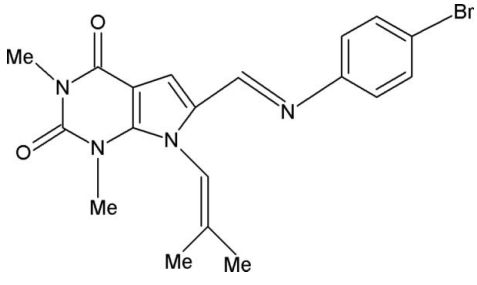
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.042; wR factor = 0.147; data-to-parameter ratio = 29.3.

In the title compound, $C_{20}H_{21}BrN_4O_2$, the pyrrolopyrimidine ring system is essentially planar. The bromophenyl ring forms a dihedral angle of 33.1 (1)° with the pyrrolopyrimidine ring system. C—H···N hydrogen bonds link the molecules into cyclic centrosymmetric $R_2^2(18)$ dimers, which are crosslinked along the [$\bar{1}$10] direction through C—H···O hydrogen bonds.

Related literature

For biological activities of pyrrolo[2,3-*d*]pyrimidine compounds, see: Hutzenlaub *et al.* (1972); Oghi *et al.* (1979); Smith *et al.* (1972); Tolman *et al.* (1968).



Experimental

Crystal data

$C_{20}H_{21}BrN_4O_2$
M_r = 429.32
Triclinic, $P\bar{1}$
a = 9.202 (3) Å
b = 9.989 (3) Å
c = 10.454 (4) Å
α = 87.363 (19)°
β = 80.67 (2)°
γ = 84.187 (19)°
V = 942.9 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.20 mm^{-1}
T = 293 (2) K
0.25 × 0.20 × 0.18 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.595, T_{max} = 0.673
25023 measured reflections
7255 independent reflections
4235 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.147
S = 1.01
7255 reflections
248 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.05 e Å^{-3}
$\Delta\rho_{min}$ = −0.68 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8A···N1^{i}	0.96	2.59	3.508 (3)	160
C9—H9B···O2	0.96	2.24	2.695 (3)	108
C10—H10A···N1	0.97	2.28	3.015 (3)	131
C20—H20···O1^{ii}	0.93	2.36	3.274 (3)	167

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ZORTEP* (Zsolnai, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

The authors thank Dr Babu Varghese, SAIF, IIT, Chennai, India, for the X-ray data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2465).

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supplementary materials

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6-[(4-Bromophenyl)iminomethyl]-1,3-dimethyl-7-(2-methylpropenyl)-1,2,3,4-tetrahydro-7*H*-pyrrolo[2,3-*d*]pyrimidine-2,4-dione

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Comment

Pyrrolo[2,3-*d*]pyrimidines are an important class of compounds that are structurally and chemically related to nucleosides and some antibiotics (Oghi *et al.*, 1979; Tolman *et al.*, 1968). The well known biological activity of these compounds has led to intense investigation of their use as antitumor, anti-allergic, antiviral and anti-inflammatory agents (Hutzenlaub *et al.*, 1972; Smith *et al.*, 1972). In view of this biological importance, the crystal structure of the title compound has been determined and the results are presnted here.

In the title molecule (Fig. 1) the pyrrolopyrimidine ring system is essentially planar, with a maximum deviation of 0.059 (2) Å for atom N3. The keto atoms O1 and O2 deviate by 0.125 (2) and 0.057 (2) Å, respectively, from the pyrimidine ring. The bromophenyl ring forms a dihedral angle of 33.1 (1)° with the pyrrolopyrimidine ring system. The Br atom deviates from the plane of the attached ring by 0.047 (1) Å.

The crystal packing is stabilized by C—H···O and C—H···N type hydrogen bonds (Table 1). Atom C20 in the molecule at (*x*, *y*, *z*) donate one proton to atom O1 at (−1 + *x*, 1 + *y*, *z*) forming a zig zag chain C(11) along the [$\bar{1}$ 1 0] direction. The molecules at (*x*, *y*, *z*) and (1 − *x*, −*y*, −*z*) are linked by C8—H8A···N1 hydrogen bonds into cyclic centrosymmetric $R^2_2(18)$ dimers.

Experimental

A mixture of 1,3-dimethyl-7-(3-methyl-but-2-enyl)-2,4-dioxo-1*H*-pyrrole (2,3 − d)pyrmidine-6-carbaldehyde (1 mmol) and *p*-bromoaniline (1 mmol) was refluxed in ethanol (10 ml) for 2 h. After cooling the solution, the precipitate formed was filtered off and washed with ethanol to give a pure yellow solid. Single crystals of the title compound suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

Refinement

H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and allowed to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C). A rotating group model was used for the methyl groups.

Figures

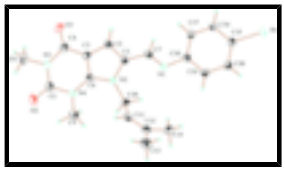


Fig. 1. The molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

6-[(4-Bromophenyl)iminomethyl]-1,3-dimethyl-7-(2-methylpropenyl)-1,2,3,4- tetrahydro-7*H*-pyrrolo[2,3-*d*]pyrimidine-2,4-dione

Crystal data

$C_{20}H_{21}BrN_4O_2$	$Z = 2$
$M_r = 429.32$	$F_{000} = 440$
Triclinic, $P\overline{1}$	$D_x = 1.512$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.202$ (3) Å	Cell parameters from 4856 reflections
$b = 9.989$ (3) Å	$\theta = 2$–33.7º
$c = 10.454$ (4) Å	$\mu = 2.20$ mm^{-1}
$\alpha = 87.363$ (19)º	$T = 293$ (2) K
$\beta = 80.67$ (2)º	Block, yellow
$\gamma = 84.187$ (19)º	0.25 × 0.20 × 0.18 mm
$V = 942.9$ (6) Å^3	

Data collection

Bruker APEXII CCD area-detector diffractometer	7255 independent reflections
Radiation source: fine-focus sealed tube	4235 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.036$
$T = 293(2)$ K	$\theta_{max} = 33.7$º
ω and φ scans	$\theta_{min} = 2.0$º
Absorption correction: multi-scan (SADABS; Sheldrick, 2001)	$h = -14\rightarrow14$
$T_{min} = 0.595$, $T_{max} = 0.673$	$k = -15\rightarrow15$
25023 measured reflections	$l = -14\rightarrow16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.042$	H-atom parameters constrained
$wR(F^2) = 0.147$	$w = 1/[\sigma^2(F_o^2) + (0.077P)^2 + 0.1592P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.001$
7255 reflections	$\Delta\rho_{max} = 1.05$ e Å^{-3}
248 parameters	$\Delta\rho_{min} = -0.67$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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}
Br	−0.31222 (3)	0.56793 (3)	−0.43672 (2)	0.06218 (12)
O1	0.49380 (19)	−0.31916 (16)	−0.03864 (18)	0.0537 (4)
O2	0.5675 (2)	−0.1746 (2)	0.34797 (19)	0.0676 (5)
N1	0.04816 (19)	0.25040 (18)	−0.06728 (17)	0.0402 (4)
N2	0.24412 (17)	0.08034 (16)	0.10161 (16)	0.0341 (3)
N3	0.51882 (19)	−0.25241 (18)	0.1613 (2)	0.0444 (4)
N4	0.41031 (19)	−0.03963 (18)	0.24052 (17)	0.0394 (4)
C1	0.2032 (2)	0.05049 (19)	−0.01682 (19)	0.0357 (4)
C2	0.2768 (2)	−0.07013 (19)	−0.05594 (19)	0.0387 (4)
H2	0.2701	−0.1133	−0.1314	0.046*
C3	0.3637 (2)	−0.11688 (19)	0.03721 (19)	0.0355 (4)
C4	0.4618 (2)	−0.2366 (2)	0.0448 (2)	0.0397 (4)
C5	0.5032 (2)	−0.1569 (2)	0.2555 (2)	0.0463 (5)
C6	0.3406 (2)	−0.02355 (19)	0.13358 (18)	0.0332 (4)
C7	0.1079 (2)	0.1321 (2)	−0.0913 (2)	0.0383 (4)
H7	0.0877	0.0942	−0.1654	0.046*
C8	0.6116 (3)	−0.3776 (3)	0.1821 (3)	0.0595 (6)
H8A	0.7129	−0.3662	0.1473	0.089*
H8B	0.5793	−0.4496	0.1393	0.089*
H8C	0.6032	−0.3988	0.2734	0.089*
C9	0.4161 (3)	0.0690 (3)	0.3280 (2)	0.0518 (5)
H9A	0.4493	0.1465	0.2784	0.078*
H9B	0.4836	0.0401	0.3871	0.078*
H9C	0.3193	0.0917	0.3760	0.078*
C10	0.1651 (2)	0.18875 (19)	0.18428 (19)	0.0371 (4)
H10A	0.1207	0.2582	0.1309	0.045*
H10B	0.2347	0.2290	0.2277	0.045*
C11	0.0472 (2)	0.1348 (2)	0.2832 (2)	0.0414 (4)
H11	0.0700	0.0514	0.3222	0.050*
C12	−0.0866 (2)	0.1957 (2)	0.3201 (2)	0.0453 (5)
C13	−0.1929 (3)	0.1296 (4)	0.4228 (3)	0.0716 (8)
H13A	−0.1501	0.0415	0.4443	0.107*
H13B	−0.2836	0.1222	0.3906	0.107*

H13C	−0.2126	0.1830	0.4988	0.107*
C14	−0.1424 (3)	0.3286 (3)	0.2669 (3)	0.0596 (6)
H14A	−0.0719	0.3563	0.1950	0.089*
H14B	−0.1560	0.3942	0.3332	0.089*
H14C	−0.2351	0.3209	0.2383	0.089*
C15	−0.1998 (2)	0.4639 (2)	−0.3244 (2)	0.0413 (4)
C16	−0.0756 (3)	0.3820 (2)	−0.3740 (2)	0.0469 (5)
H16	−0.0476	0.3755	−0.4632	0.056*
C17	0.0068 (2)	0.3100 (2)	−0.2911 (2)	0.0441 (5)
H17	0.0906	0.2550	−0.3248	0.053*
C18	−0.0334 (2)	0.3183 (2)	−0.15775 (19)	0.0369 (4)
C19	−0.1572 (2)	0.4033 (2)	−0.1098 (2)	0.0412 (4)
H19	−0.1837	0.4118	−0.0207	0.049*
C20	−0.2421 (2)	0.4754 (2)	−0.1920 (2)	0.0416 (4)
H20	−0.3260	0.5306	−0.1588	0.050*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br	0.06096 (17)	0.0752 (2)	0.04937 (16)	0.01901 (12)	−0.02074 (12)	−0.00422 (12)
O1	0.0550 (9)	0.0442 (8)	0.0581 (10)	0.0067 (7)	−0.0018 (8)	−0.0130 (7)
O2	0.0726 (12)	0.0725 (12)	0.0623 (12)	0.0100 (10)	−0.0351 (10)	−0.0007 (10)
N1	0.0431 (9)	0.0411 (9)	0.0366 (9)	−0.0006 (7)	−0.0089 (7)	0.0002 (7)
N2	0.0369 (8)	0.0329 (8)	0.0325 (8)	−0.0030 (6)	−0.0053 (6)	−0.0026 (6)
N3	0.0374 (8)	0.0386 (9)	0.0562 (11)	−0.0003 (7)	−0.0076 (8)	0.0026 (8)
N4	0.0402 (8)	0.0421 (9)	0.0368 (9)	−0.0023 (7)	−0.0089 (7)	−0.0039 (7)
C1	0.0384 (9)	0.0332 (9)	0.0364 (10)	−0.0060 (7)	−0.0069 (7)	−0.0020 (7)
C2	0.0454 (10)	0.0362 (10)	0.0354 (10)	−0.0054 (8)	−0.0066 (8)	−0.0051 (8)
C3	0.0366 (9)	0.0316 (9)	0.0376 (10)	−0.0036 (7)	−0.0025 (7)	−0.0043 (7)
C4	0.0344 (9)	0.0356 (9)	0.0468 (11)	−0.0028 (7)	−0.0006 (8)	−0.0007 (8)
C5	0.0397 (10)	0.0486 (12)	0.0506 (13)	−0.0021 (9)	−0.0103 (9)	0.0057 (10)
C6	0.0329 (8)	0.0340 (9)	0.0328 (9)	−0.0049 (7)	−0.0042 (7)	−0.0012 (7)
C7	0.0409 (10)	0.0386 (10)	0.0371 (10)	−0.0067 (8)	−0.0096 (8)	−0.0007 (8)
C8	0.0475 (12)	0.0471 (13)	0.0834 (19)	0.0064 (10)	−0.0178 (12)	0.0070 (12)
C9	0.0542 (13)	0.0599 (14)	0.0454 (12)	−0.0036 (11)	−0.0182 (10)	−0.0120 (11)
C10	0.0406 (9)	0.0336 (9)	0.0371 (10)	−0.0017 (7)	−0.0053 (8)	−0.0073 (8)
C11	0.0443 (10)	0.0470 (11)	0.0331 (10)	−0.0031 (8)	−0.0072 (8)	−0.0018 (8)
C12	0.0423 (10)	0.0605 (13)	0.0343 (10)	−0.0052 (9)	−0.0062 (8)	−0.0130 (9)
C13	0.0525 (14)	0.107 (2)	0.0539 (16)	−0.0189 (15)	0.0031 (12)	−0.0057 (16)
C14	0.0554 (14)	0.0665 (16)	0.0545 (14)	0.0128 (11)	−0.0081 (11)	−0.0194 (12)
C15	0.0417 (10)	0.0429 (10)	0.0405 (11)	0.0006 (8)	−0.0123 (8)	−0.0035 (8)
C16	0.0520 (12)	0.0543 (13)	0.0328 (10)	0.0060 (10)	−0.0067 (9)	−0.0070 (9)
C17	0.0434 (10)	0.0480 (11)	0.0380 (11)	0.0072 (8)	−0.0043 (8)	−0.0051 (9)
C18	0.0379 (9)	0.0373 (9)	0.0362 (10)	−0.0040 (7)	−0.0081 (7)	−0.0011 (8)
C19	0.0448 (10)	0.0426 (10)	0.0346 (10)	−0.0005 (8)	−0.0031 (8)	−0.0030 (8)
C20	0.0370 (9)	0.0417 (10)	0.0443 (11)	0.0019 (8)	−0.0033 (8)	−0.0048 (9)

Geometric parameters (Å, °)

Br—C15	1.895 (2)	C9—H9B	0.96
O1—C4	1.209 (3)	C9—H9C	0.96
O2—C5	1.210 (3)	C10—C11	1.497 (3)
N1—C7	1.270 (3)	C10—H10A	0.97
N1—C18	1.409 (3)	C10—H10B	0.97
N2—C6	1.362 (3)	C11—C12	1.324 (3)
N2—C1	1.404 (3)	C11—H11	0.93
N2—C10	1.473 (2)	C12—C14	1.490 (4)
N3—C5	1.383 (3)	C12—C13	1.507 (4)
N3—C4	1.399 (3)	C13—H13A	0.96
N3—C8	1.469 (3)	C13—H13B	0.96
N4—C6	1.372 (3)	C13—H13C	0.96
N4—C5	1.397 (3)	C14—H14A	0.96
N4—C9	1.461 (3)	C14—H14B	0.96
C1—C2	1.367 (3)	C14—H14C	0.96
C1—C7	1.435 (3)	C15—C16	1.380 (3)
C2—C3	1.393 (3)	C15—C20	1.383 (3)
C2—H2	0.93	C16—C17	1.374 (3)
C3—C6	1.381 (3)	C16—H16	0.93
C3—C4	1.431 (3)	C17—C18	1.387 (3)
C7—H7	0.93	C17—H17	0.93
C8—H8A	0.96	C18—C19	1.389 (3)
C8—H8B	0.96	C19—C20	1.383 (3)
C8—H8C	0.96	C19—H19	0.93
C9—H9A	0.96	C20—H20	0.93
C7—N1—C18	118.68 (18)	N2—C10—C11	110.60 (16)
C6—N2—C1	107.35 (15)	N2—C10—H10A	109.5
C6—N2—C10	128.39 (17)	C11—C10—H10A	109.5
C1—N2—C10	122.74 (16)	N2—C10—H10B	109.5
C5—N3—C4	125.68 (18)	C11—C10—H10B	109.5
C5—N3—C8	116.8 (2)	H10A—C10—H10B	108.1
C4—N3—C8	117.4 (2)	C12—C11—C10	125.6 (2)
C6—N4—C5	119.08 (18)	C12—C11—H11	117.2
C6—N4—C9	123.49 (18)	C10—C11—H11	117.2
C5—N4—C9	116.40 (18)	C11—C12—C14	124.4 (2)
C2—C1—N2	108.19 (18)	C11—C12—C13	119.5 (2)
C2—C1—C7	123.93 (19)	C14—C12—C13	116.1 (2)
N2—C1—C7	127.80 (18)	C12—C13—H13A	109.5
C1—C2—C3	107.90 (18)	C12—C13—H13B	109.5
C1—C2—H2	126.0	H13A—C13—H13B	109.5
C3—C2—H2	126.0	C12—C13—H13C	109.5
C2—C3—C6	107.51 (17)	H13A—C13—H13C	109.5
C2—C3—C4	131.28 (18)	H13B—C13—H13C	109.5
C6—C3—C4	121.21 (19)	C12—C14—H14A	109.5
O1—C4—N3	121.5 (2)	C12—C14—H14B	109.5
O1—C4—C3	125.0 (2)	H14A—C14—H14B	109.5

N3—C4—C3	113.50 (18)	C12—C14—H14C	109.5
O2—C5—N3	121.1 (2)	H14A—C14—H14C	109.5
O2—C5—N4	121.2 (2)	H14B—C14—H14C	109.5
N3—C5—N4	117.76 (19)	C16—C15—C20	120.8 (2)
N2—C6—N4	128.68 (17)	C16—C15—Br	120.57 (17)
N2—C6—C3	109.05 (17)	C20—C15—Br	118.62 (16)
N4—C6—C3	122.26 (18)	C17—C16—C15	119.8 (2)
N1—C7—C1	127.14 (19)	C17—C16—H16	120.1
N1—C7—H7	116.4	C15—C16—H16	120.1
C1—C7—H7	116.4	C16—C17—C18	120.89 (19)
N3—C8—H8A	109.5	C16—C17—H17	119.6
N3—C8—H8B	109.5	C18—C17—H17	119.6
H8A—C8—H8B	109.5	C19—C18—C17	118.45 (19)
N3—C8—H8C	109.5	C19—C18—N1	117.60 (18)
H8A—C8—H8C	109.5	C17—C18—N1	123.88 (18)
H8B—C8—H8C	109.5	C18—C19—C20	121.3 (2)
N4—C9—H9A	109.5	C18—C19—H19	119.3
N4—C9—H9B	109.5	C20—C19—H19	119.3
H9A—C9—H9B	109.5	C19—C20—C15	118.77 (19)
N4—C9—H9C	109.5	C19—C20—H20	120.6
H9A—C9—H9C	109.5	C15—C20—H20	120.6
H9B—C9—H9C	109.5		
C6—N2—C1—C2	−0.8 (2)	C5—N4—C6—N2	178.48 (19)
C10—N2—C1—C2	−167.79 (17)	C9—N4—C6—N2	−13.6 (3)
C6—N2—C1—C7	−177.54 (19)	C5—N4—C6—C3	−2.7 (3)
C10—N2—C1—C7	15.5 (3)	C9—N4—C6—C3	165.21 (19)
N2—C1—C2—C3	0.2 (2)	C2—C3—C6—N2	−1.0 (2)
C7—C1—C2—C3	177.07 (18)	C4—C3—C6—N2	179.45 (17)
C1—C2—C3—C6	0.5 (2)	C2—C3—C6—N4	179.97 (17)
C1—C2—C3—C4	180.0 (2)	C4—C3—C6—N4	0.4 (3)
C5—N3—C4—O1	171.9 (2)	C18—N1—C7—C1	175.24 (19)
C8—N3—C4—O1	−3.9 (3)	C2—C1—C7—N1	−172.4 (2)
C5—N3—C4—C3	−8.8 (3)	N2—C1—C7—N1	3.8 (3)
C8—N3—C4—C3	175.42 (19)	C6—N2—C10—C11	−71.1 (2)
C2—C3—C4—O1	4.8 (4)	C1—N2—C10—C11	93.0 (2)
C6—C3—C4—O1	−175.78 (19)	N2—C10—C11—C12	−139.8 (2)
C2—C3—C4—N3	−174.5 (2)	C10—C11—C12—C14	0.8 (3)
C6—C3—C4—N3	4.9 (3)	C10—C11—C12—C13	−179.0 (2)
C4—N3—C5—O2	−173.2 (2)	C20—C15—C16—C17	0.5 (4)
C8—N3—C5—O2	2.6 (3)	Br—C15—C16—C17	178.26 (18)
C4—N3—C5—N4	6.9 (3)	C15—C16—C17—C18	0.1 (4)
C8—N3—C5—N4	−177.27 (19)	C16—C17—C18—C19	−1.3 (3)
C6—N4—C5—O2	179.5 (2)	C16—C17—C18—N1	−178.1 (2)
C9—N4—C5—O2	10.7 (3)	C7—N1—C18—C19	145.2 (2)
C6—N4—C5—N3	−0.7 (3)	C7—N1—C18—C17	−38.0 (3)
C9—N4—C5—N3	−169.48 (19)	C17—C18—C19—C20	1.9 (3)
C1—N2—C6—N4	−179.96 (18)	N1—C18—C19—C20	178.96 (18)
C10—N2—C6—N4	−13.9 (3)	C18—C19—C20—C15	−1.3 (3)
C1—N2—C6—C3	1.1 (2)	C16—C15—C20—C19	0.1 (3)

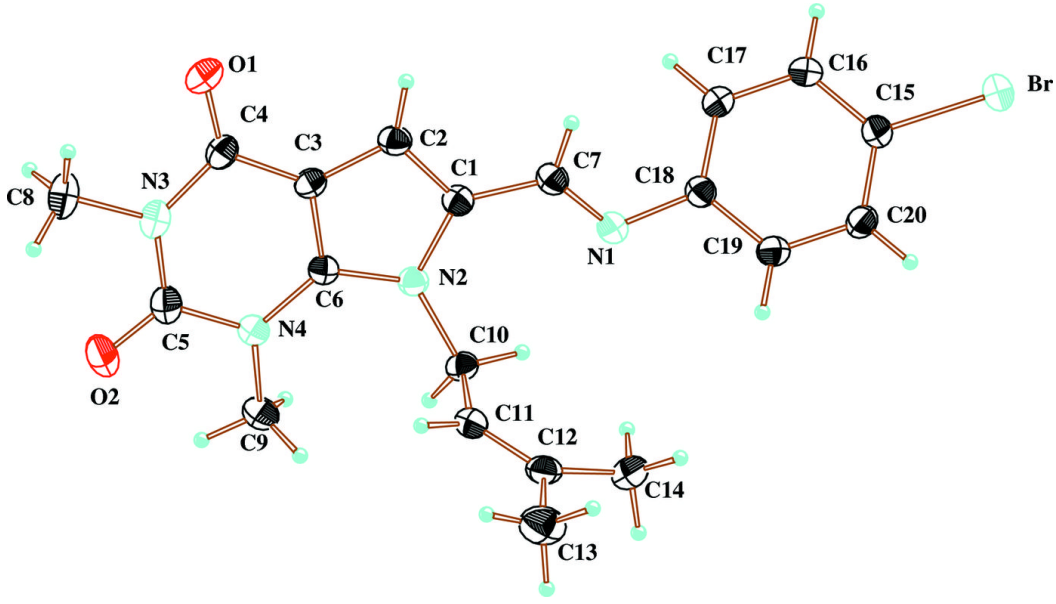
C10—N2—C6—C3	167.14 (17)	Br—C15—C20—C19	−177.71 (16)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8A···N1^{i}	0.96	2.59	3.508 (3)	160
C9—H9B···O2	0.96	2.24	2.695 (3)	108
C10—H10A···N1	0.97	2.28	3.015 (3)	131
C20—H20···O1^{ii}	0.93	2.36	3.274 (3)	167

Symmetry codes: (i) −*x*+1, −*y*, −*z*; (ii) *x*−1, *y*+1, *z*.

Fig. 1


O1
C4
C3
C2
C1
C7
C17
C16
C15
Br
C8
N3
C18
C20
N1
C19
N2
C6
C5
N4
C10
O2
C11
C9
C12
C14
C13