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2-(1*H*-1,2,3-Benzotriazol-1-yl)-1-benzoylethyl 4-methylbenzoate

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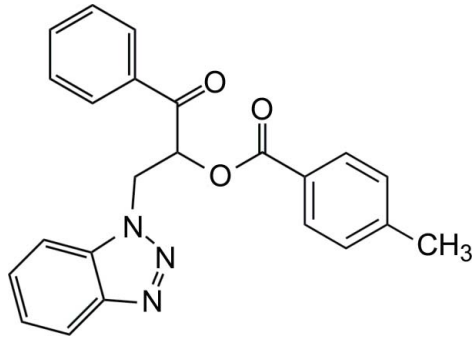
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.004 Å; R factor = 0.049; wR factor = 0.140; data-to-parameter ratio = 15.2.

In the crystal structure of the title compound, $C_{23}H_{19}N_3O_3$, molecules are linked into chains parallel to the c axis by C—H···O hydrogen bonds. Adjacent chains are assembled into two-dimensional layers *via* C—H···N hydrogen bonds. The packing is further stabilized by π–π interactions between triazole and phenyl rings.

Related literature

For a general background on the pharmacological activities of benzotriazoles, see: Chen & Wu (2005). For related literature, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{23}H_{19}N_3O_3$
M_r = 385.41
Monoclinic, $C2/c$
a = 20.376 (4) Å
b = 19.648 (4) Å
c = 10.213 (2) Å
β = 107.605 (4)°
V = 3897.3 (13) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 294 (2) K
0.22 × 0.18 × 0.12 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.981, T_{max} = 0.989
11106 measured reflections
3994 independent reflections
2014 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.140
S = 1.00
3994 reflections
263 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O1^{i}	0.93	2.50	3.157 (3)	128
C7—H7A···N2^{ii}	0.97	2.59	3.560 (3)	176
C18—H18···O3^{iii}	0.93	2.51	3.317 (3)	145

Symmetry codes: (i) $x, -y, z+\frac{1}{2}$; (ii) $-x+\frac{1}{2}, -y+\frac{1}{2}, -z+2$; (iii) $-x, -y, -z+1$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2151).

References

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supplementary materials

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2-(1*H*-1,2,3-Benzotriazol-1-yl)-1-benzoylethyl 4-methylbenzoate

W.-L. Zeng, Y.-C. Zhang and Y.-M. Hong

Comment

1*H*-Benzotriazole and its derivatives are an important class of compounds because they exhibit a broad spectrum of pharmacological activities such as antifungal, antitumor and antineoplastic activities (Chen & Wu, 2005). We report here the synthesis and crystal structure of the title compound as part of our ongoing studies on new benzotriazole compounds with higher bioactivity.

In the title compound (Fig. 1), all bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The benzotriazole ring system is essentially planar, with a dihedral angle of 2.67 (1)° between the triazole ring (atoms N1—N3/C1/C6) and the benzene ring (C1—C6). The dihedral angles between the mean planes of the benzotriazole system and the six-membered aromatic rings C10—C15 and C17—C22 are 6.85 (1) and 66.06 (1)°, respectively. The dihedral angle between these two latter rings is 61.7 (2)°. In the crystal structure, intermolecular C—H···O hydrogen bonds (Table1) link the molecules into chains running parallel to the *c* axis. Adjacent chains are assembled into two-dimensional layers *via* C—H···N hydrogen bonds (Fig. 2). The packing is further stabilized by π···π interactions occurring between symmetry-related triazole and phenyl rings [$Cg1\cdots Cg2^{i}$ = 3.578 (3) Å; perpendicular interplanar distance = 3.568 (3) Å; *Cg*1 and *Cg*2 are the centroids of the N1—N3/C1/C6 triazole ring and C10—C15 phenyl ring, respectively; symmetry code: (i) 1/2 − *x*, 1/2 − *y*, 2 − *z*].

Experimental

Bromine (3.2 g, 0.02 mol) was added dropwise to a solution of 3-(1*H*-benzo[*d*][1,2,3]triazol-1-yl)-1-phenylpropan-1-one (5.0 g, 0.02 mol) and sodium acetate (1.6 g, 0.02 mol) in acetic acid (50 ml). The reaction proceeded for 7 h. Water (50 ml) and chloroform (20 ml) were then added. The organic layer was washed successively with a saturated sodium bicarbonate solution and brine, dried over anhydrous magnesium sulfate and the chloroform solution filtered. This fraction was cooled with ice-water, then a solution of 4-methylbenzoic acid (2.7 g, 0.02 mol) in acetone (10 ml) and triethylamine (2.8 ml) was added. The mixture was stirred with ice-water for about 6 h. The solution was then filtered and concentrated. Single crystals suitable for X-ray analysis were obtained by slow evaporation of an acetone-ethylacetate (1:1 *v*/*v*) solution at room temperature over a period of one week.

Refinement

All H atoms were located in difference Fourier maps and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with U_{iso}(H) = 1.2 U_{eq}(C) or 1.5 U_{eq}(C) for the methyl group.

Figures

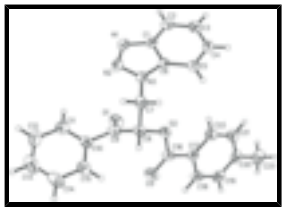

Fig. 1. The molecular structure of title compound with 30% probability ellipsoids.

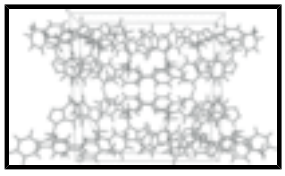

Fig. 2. Packing diagram of the title compound viewed along the *c* axis. Intermolecular hydrogen bonds are shown as dashed lines.

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Crystal data

$C_{23}H_{19}N_3O_3$	F_{000} = 1616
M_r = 385.41	D_x = 1.314 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 1885 reflections
a = 20.376 (4) Å	θ = 2.3–22.6º
b = 19.648 (4) Å	μ = 0.09 mm^{-1}
c = 10.213 (2) Å	*T* = 294 (2) K
β = 107.605 (4)º	Block, colourless
V = 3897.3 (13) Å^3	0.22 × 0.18 × 0.12 mm
Z = 8	

Data collection

Siemens SMART CCD area-detector diffractometer	3994 independent reflections
Radiation source: fine-focus sealed tube	2014 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.046
T = 294(2) K	θ_{max} = 26.4º
φ and ω scans	θ_{min} = 1.5º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −16→25
T_{min} = 0.981, T_{max} = 0.989	*k* = −24→20
11106 measured reflections	*l* = −12→9

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.049$	H-atom parameters constrained
$wR(F^2) = 0.140$	$w = 1/[\sigma^2(F_o^2) + (0.063P)^2 + 0.064P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.004$
3994 reflections	$\Delta\rho_{max} = 0.26$ e Å^{-3}
263 parameters	$\Delta\rho_{min} = -0.17$ 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 $F^2 > 2$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}
O1	0.20658 (8)	0.12677 (8)	0.70219 (18)	0.0703 (5)
O2	0.14502 (7)	0.05617 (7)	0.86281 (16)	0.0550 (4)
O3	0.05904 (9)	0.06461 (9)	0.6674 (2)	0.0879 (6)
N1	0.36982 (10)	0.14012 (10)	1.0086 (2)	0.0598 (5)
N2	0.30975 (10)	0.16959 (9)	0.9822 (2)	0.0581 (5)
N3	0.26645 (9)	0.12819 (9)	1.02305 (18)	0.0471 (5)
C1	0.36587 (11)	0.07846 (11)	1.0694 (2)	0.0475 (6)
C2	0.41650 (11)	0.02937 (13)	1.1214 (3)	0.0624 (7)
H2	0.4608	0.0342	1.1146	0.075*
C3	0.39807 (13)	−0.02585 (13)	1.1825 (3)	0.0703 (8)
H3	0.4306	−0.0596	1.2180	0.084*
C4	0.33142 (12)	−0.03349 (12)	1.1938 (3)	0.0648 (7)
H4	0.3213	−0.0718	1.2377	0.078*
C5	0.28111 (11)	0.01386 (11)	1.1421 (2)	0.0538 (6)
H5	0.2368	0.0086	1.1482	0.065*
C6	0.30000 (10)	0.07063 (10)	1.0794 (2)	0.0431 (5)
C7	0.19630 (11)	0.14953 (11)	1.0045 (2)	0.0542 (6)
H7A	0.1953	0.1987	1.0130	0.065*
H7B	0.1808	0.1300	1.0773	0.065*
C8	0.14636 (11)	0.12887 (11)	0.8666 (2)	0.0519 (6)
H8	0.1003	0.1457	0.8609	0.062*
C9	0.16798 (11)	0.15841 (12)	0.7499 (2)	0.0524 (6)
C10	0.14402 (11)	0.22827 (11)	0.7005 (2)	0.0500 (6)
C11	0.18920 (13)	0.27258 (14)	0.6695 (3)	0.0662 (7)

H11	0.2345	0.2593	0.6824	0.079*
C12	0.16787 (18)	0.33635 (15)	0.6197 (3)	0.0817 (9)
H12	0.1990	0.3665	0.6008	0.098*
C13	0.1012 (2)	0.35565 (15)	0.5977 (3)	0.0873 (10)
H13	0.0868	0.3988	0.5632	0.105*
C14	0.05536 (15)	0.31160 (16)	0.6266 (3)	0.0809 (9)
H14	0.0097	0.3245	0.6106	0.097*
C15	0.07713 (12)	0.24794 (13)	0.6795 (3)	0.0642 (7)
H15	0.0463	0.2183	0.7009	0.077*
C16	0.09767 (11)	0.02871 (13)	0.7527 (3)	0.0605 (7)
C17	0.09855 (10)	−0.04588 (12)	0.7526 (2)	0.0522 (6)
C18	0.05402 (11)	−0.08051 (14)	0.6424 (2)	0.0627 (7)
H18	0.0250	−0.0563	0.5694	0.075*
C19	0.05285 (12)	−0.15056 (14)	0.6412 (3)	0.0636 (7)
H19	0.0227	−0.1730	0.5670	0.076*
C20	0.09510 (12)	−0.18837 (13)	0.7469 (3)	0.0597 (7)
C21	0.13932 (12)	−0.15321 (13)	0.8558 (3)	0.0611 (6)
H21	0.1684	−0.1776	0.9284	0.073*
C22	0.14135 (12)	−0.08347 (12)	0.8595 (2)	0.0597 (7)
H22	0.1716	−0.0613	0.9340	0.072*
C23	0.09377 (14)	−0.26485 (13)	0.7461 (3)	0.0859 (9)
H23A	0.1385	−0.2819	0.7507	0.129*
H23B	0.0607	−0.2806	0.6632	0.129*
H23C	0.0812	−0.2809	0.8241	0.129*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0719 (11)	0.0785 (12)	0.0655 (12)	0.0248 (9)	0.0282 (10)	0.0047 (9)
O2	0.0508 (9)	0.0517 (10)	0.0530 (11)	−0.0020 (7)	0.0011 (8)	0.0017 (8)
O3	0.0787 (13)	0.0800 (13)	0.0767 (14)	−0.0005 (10)	−0.0187 (10)	0.0139 (11)
N1	0.0540 (12)	0.0652 (14)	0.0566 (14)	−0.0139 (10)	0.0112 (10)	0.0065 (10)
N2	0.0613 (13)	0.0522 (12)	0.0573 (14)	−0.0143 (10)	0.0124 (10)	0.0042 (10)
N3	0.0496 (11)	0.0458 (11)	0.0425 (12)	−0.0046 (9)	0.0087 (9)	−0.0003 (9)
C1	0.0451 (13)	0.0523 (14)	0.0410 (14)	−0.0127 (11)	0.0065 (10)	−0.0011 (11)
C2	0.0433 (13)	0.0721 (18)	0.0647 (18)	−0.0037 (13)	0.0059 (12)	0.0003 (14)
C3	0.0598 (17)	0.0604 (17)	0.077 (2)	0.0031 (13)	0.0007 (14)	0.0091 (14)
C4	0.0644 (17)	0.0558 (16)	0.0639 (18)	−0.0124 (13)	0.0040 (13)	0.0122 (13)
C5	0.0488 (13)	0.0560 (15)	0.0517 (16)	−0.0076 (12)	0.0079 (11)	0.0042 (12)
C6	0.0437 (12)	0.0437 (13)	0.0363 (13)	−0.0070 (10)	0.0037 (10)	−0.0021 (10)
C7	0.0607 (15)	0.0494 (14)	0.0532 (16)	0.0033 (11)	0.0182 (12)	0.0002 (11)
C8	0.0467 (13)	0.0529 (15)	0.0520 (16)	0.0078 (11)	0.0087 (11)	0.0023 (12)
C9	0.0439 (13)	0.0620 (16)	0.0468 (15)	0.0083 (12)	0.0072 (11)	−0.0041 (12)
C10	0.0558 (14)	0.0502 (14)	0.0396 (14)	0.0047 (12)	0.0079 (11)	−0.0036 (11)
C11	0.0646 (16)	0.0695 (18)	0.0588 (17)	−0.0023 (14)	0.0101 (13)	−0.0005 (14)
C12	0.111 (3)	0.065 (2)	0.068 (2)	−0.0196 (18)	0.0262 (18)	−0.0009 (16)
C13	0.136 (3)	0.0563 (18)	0.062 (2)	0.024 (2)	0.019 (2)	0.0025 (15)
C14	0.084 (2)	0.084 (2)	0.070 (2)	0.0360 (18)	0.0181 (16)	0.0020 (17)

C15	0.0630 (16)	0.0662 (17)	0.0630 (18)	0.0133 (13)	0.0183 (13)	0.0049 (14)
C16	0.0463 (14)	0.0723 (19)	0.0525 (17)	−0.0045 (13)	−0.0007 (12)	0.0066 (14)
C17	0.0469 (13)	0.0599 (16)	0.0456 (15)	−0.0069 (11)	0.0074 (11)	0.0016 (12)
C18	0.0523 (15)	0.079 (2)	0.0481 (16)	−0.0104 (13)	0.0026 (12)	0.0011 (13)
C19	0.0606 (16)	0.079 (2)	0.0513 (17)	−0.0233 (14)	0.0168 (13)	−0.0140 (14)
C20	0.0667 (16)	0.0667 (17)	0.0547 (17)	−0.0143 (13)	0.0319 (14)	−0.0076 (14)
C21	0.0711 (17)	0.0628 (17)	0.0472 (16)	−0.0055 (13)	0.0145 (13)	−0.0017 (13)
C22	0.0612 (15)	0.0623 (17)	0.0468 (16)	−0.0076 (12)	0.0033 (12)	−0.0037 (13)
C23	0.106 (2)	0.071 (2)	0.090 (2)	−0.0212 (16)	0.0433 (18)	−0.0181 (16)

Geometric parameters (Å, °)

O1—C9	1.214 (2)	C10—C11	1.372 (3)
O2—C16	1.353 (3)	C11—C12	1.373 (4)
O2—C8	1.429 (2)	C11—H11	0.9300
O3—C16	1.209 (3)	C12—C13	1.362 (4)
N1—N2	1.306 (2)	C12—H12	0.9300
N1—C1	1.375 (3)	C13—C14	1.369 (4)
N2—N3	1.356 (2)	C13—H13	0.9300
N3—C6	1.356 (3)	C14—C15	1.381 (4)
N3—C7	1.446 (3)	C14—H14	0.9300
C1—C6	1.385 (3)	C15—H15	0.9300
C1—C2	1.395 (3)	C16—C17	1.466 (3)
C2—C3	1.360 (3)	C17—C22	1.386 (3)
C2—H2	0.9300	C17—C18	1.391 (3)
C3—C4	1.405 (3)	C18—C19	1.377 (3)
C3—H3	0.9300	C18—H18	0.9300
C4—C5	1.367 (3)	C19—C20	1.377 (3)
C4—H4	0.9300	C19—H19	0.9300
C5—C6	1.397 (3)	C20—C21	1.386 (3)
C5—H5	0.9300	C20—C23	1.503 (3)
C7—C8	1.522 (3)	C21—C22	1.371 (3)
C7—H7A	0.9700	C21—H21	0.9300
C7—H7B	0.9700	C22—H22	0.9300
C8—C9	1.507 (3)	C23—H23A	0.9600
C8—H8	0.9800	C23—H23B	0.9600
C9—C10	1.493 (3)	C23—H23C	0.9600
C10—C15	1.370 (3)		
C16—O2—C8	115.11 (18)	C10—C11—C12	120.4 (2)
N2—N1—C1	107.75 (18)	C10—C11—H11	119.8
N1—N2—N3	109.08 (18)	C12—C11—H11	119.8
N2—N3—C6	109.84 (17)	C13—C12—C11	120.2 (3)
N2—N3—C7	119.70 (18)	C13—C12—H12	119.9
C6—N3—C7	130.46 (18)	C11—C12—H12	119.9
N1—C1—C6	108.76 (19)	C12—C13—C14	120.0 (3)
N1—C1—C2	130.1 (2)	C12—C13—H13	120.0
C6—C1—C2	121.1 (2)	C14—C13—H13	120.0
C3—C2—C1	116.8 (2)	C13—C14—C15	119.8 (3)
C3—C2—H2	121.6	C13—C14—H14	120.1

C1—C2—H2	121.6	C15—C14—H14	120.1
C2—C3—C4	122.1 (2)	C10—C15—C14	120.2 (3)
C2—C3—H3	119.0	C10—C15—H15	119.9
C4—C3—H3	119.0	C14—C15—H15	119.9
C5—C4—C3	121.7 (2)	O3—C16—O2	120.8 (2)
C5—C4—H4	119.1	O3—C16—C17	126.0 (2)
C3—C4—H4	119.1	O2—C16—C17	113.2 (2)
C4—C5—C6	116.3 (2)	C22—C17—C18	118.5 (2)
C4—C5—H5	121.9	C22—C17—C16	122.5 (2)
C6—C5—H5	121.9	C18—C17—C16	119.0 (2)
N3—C6—C1	104.56 (18)	C19—C18—C17	120.1 (2)
N3—C6—C5	133.4 (2)	C19—C18—H18	120.0
C1—C6—C5	122.0 (2)	C17—C18—H18	120.0
N3—C7—C8	113.69 (18)	C18—C19—C20	121.8 (2)
N3—C7—H7A	108.8	C18—C19—H19	119.1
C8—C7—H7A	108.8	C20—C19—H19	119.1
N3—C7—H7B	108.8	C19—C20—C21	117.4 (2)
C8—C7—H7B	108.8	C19—C20—C23	122.0 (2)
H7A—C7—H7B	107.7	C21—C20—C23	120.6 (3)
O2—C8—C9	111.77 (18)	C22—C21—C20	121.8 (2)
O2—C8—C7	107.09 (18)	C22—C21—H21	119.1
C9—C8—C7	110.83 (19)	C20—C21—H21	119.1
O2—C8—H8	109.0	C21—C22—C17	120.3 (2)
C9—C8—H8	109.0	C21—C22—H22	119.8
C7—C8—H8	109.0	C17—C22—H22	119.8
O1—C9—C10	121.4 (2)	C20—C23—H23A	109.5
O1—C9—C8	120.0 (2)	C20—C23—H23B	109.5
C10—C9—C8	118.51 (19)	H23A—C23—H23B	109.5
C15—C10—C11	119.3 (2)	C20—C23—H23C	109.5
C15—C10—C9	121.4 (2)	H23A—C23—H23C	109.5
C11—C10—C9	119.2 (2)	H23B—C23—H23C	109.5
C1—N1—N2—N3	−0.6 (2)	C7—C8—C9—C10	−87.0 (2)
N1—N2—N3—C6	0.9 (2)	O1—C9—C10—C15	138.4 (2)
N1—N2—N3—C7	−179.93 (18)	C8—C9—C10—C15	−44.9 (3)
N2—N1—C1—C6	0.2 (2)	O1—C9—C10—C11	−38.5 (3)
N2—N1—C1—C2	−177.3 (2)	C8—C9—C10—C11	138.1 (2)
N1—C1—C2—C3	176.8 (2)	C15—C10—C11—C12	0.9 (4)
C6—C1—C2—C3	−0.4 (3)	C9—C10—C11—C12	177.9 (2)
C1—C2—C3—C4	−0.2 (4)	C10—C11—C12—C13	−1.4 (4)
C2—C3—C4—C5	0.9 (4)	C11—C12—C13—C14	0.6 (4)
C3—C4—C5—C6	−1.0 (3)	C12—C13—C14—C15	0.8 (4)
N2—N3—C6—C1	−0.7 (2)	C11—C10—C15—C14	0.5 (4)
C7—N3—C6—C1	−179.8 (2)	C9—C10—C15—C14	−176.4 (2)
N2—N3—C6—C5	176.6 (2)	C13—C14—C15—C10	−1.3 (4)
C7—N3—C6—C5	−2.4 (4)	C8—O2—C16—O3	−1.6 (3)
N1—C1—C6—N3	0.3 (2)	C8—O2—C16—C17	179.55 (18)
C2—C1—C6—N3	178.1 (2)	O3—C16—C17—C22	−175.4 (3)
N1—C1—C6—C5	−177.4 (2)	O2—C16—C17—C22	3.4 (3)
C2—C1—C6—C5	0.3 (3)	O3—C16—C17—C18	3.5 (4)

C4—C5—C6—N3	−176.6 (2)	O2—C16—C17—C18	−177.7 (2)
C4—C5—C6—C1	0.4 (3)	C22—C17—C18—C19	0.3 (3)
N2—N3—C7—C8	89.4 (2)	C16—C17—C18—C19	−178.6 (2)
C6—N3—C7—C8	−91.6 (3)	C17—C18—C19—C20	−0.2 (4)
C16—O2—C8—C9	−65.0 (2)	C18—C19—C20—C21	0.1 (3)
C16—O2—C8—C7	173.46 (19)	C18—C19—C20—C23	179.8 (2)
N3—C7—C8—O2	63.2 (2)	C19—C20—C21—C22	0.1 (4)
N3—C7—C8—C9	−58.9 (2)	C23—C20—C21—C22	−179.7 (2)
O2—C8—C9—O1	−29.6 (3)	C20—C21—C22—C17	0.0 (4)
C7—C8—C9—O1	89.8 (3)	C18—C17—C22—C21	−0.2 (4)
O2—C8—C9—C10	153.67 (18)	C16—C17—C22—C21	178.7 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···O1^{i}	0.93	2.50	3.157 (3)	128
C7—H7A···N2^{ii}	0.97	2.59	3.560 (3)	176
C18—H18···O3^{iii}	0.93	2.51	3.317 (3)	145

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

Fig. 1

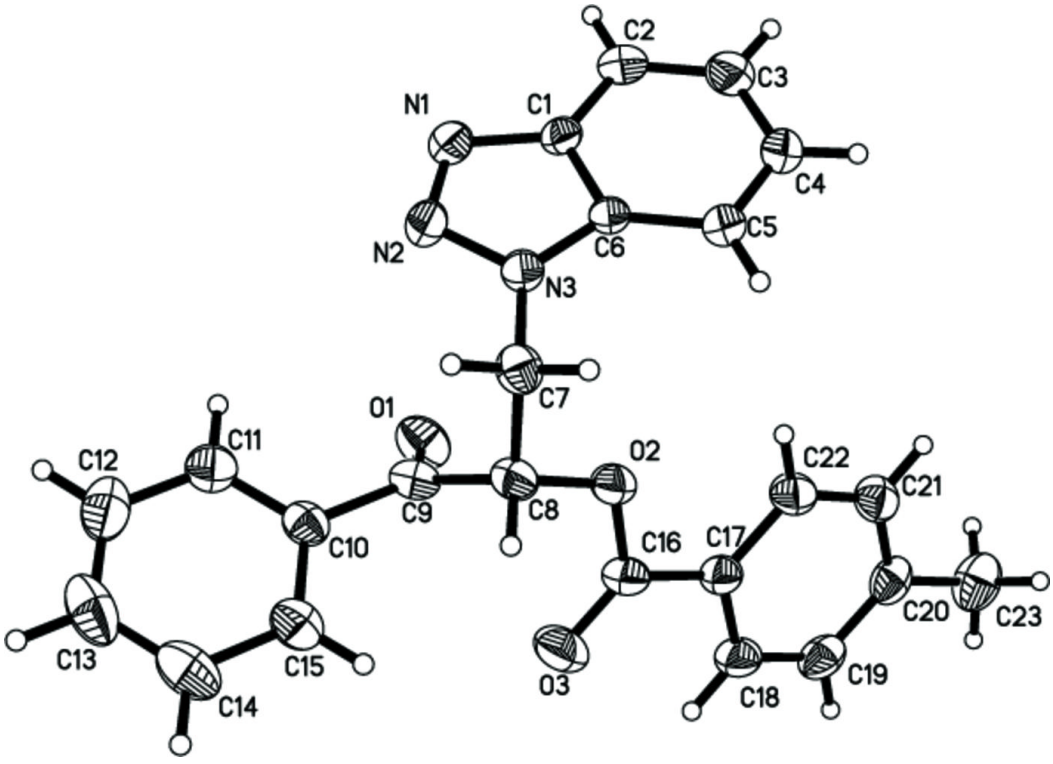
C2
C3
N1
C1
C4
C5
N2
C6
N3
C7
O1
C11
C12
O2
C22
C21
C9
C8
C10
C16
C17
C20
C23
C13
C15
O3
C19
C14
C18

Fig. 2