Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(1*H*-Benzotriazol-1-yl)-1-(3-methoxybenzoyl)ethyl isonicotinate

Wei Wang and Zhen-Hua Mei*

College of Life Science and Pharmaceutical Engineering, Nanjing University of Technology, 210009 Nanjing, Jiangsu, People's Republic of China
Correspondence e-mail: mzh62@qust.edu.cn

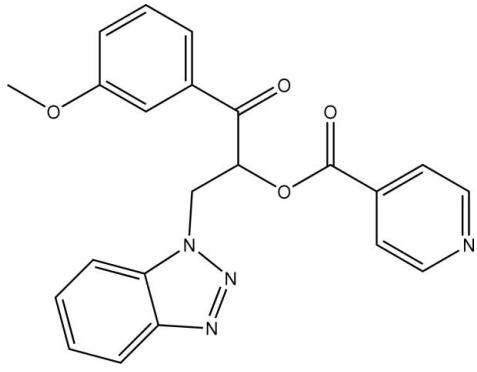
Received 5 January 2009; accepted 10 January 2009

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.046; wR factor = 0.119; data-to-parameter ratio = 14.1.

In the title compound, $C_{22}H_{18}N_4O_4$, molecules are linked to each other by C—H···N and C—H···O intermolecular hydrogen-bonding interactions. The crystal packing is further stabilized by C—H···π, and π–π interactions with a distance of 3.783 (3) Å between the centroids of the benzene rings of the benzotriazole system.

Related literature

For general background on benzotriazole and its derivatives, see: Chen & Wu (2005). For details of the synthesis, see: Wan *et al.* (2006). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{22}H_{18}N_4O_4$
M_r = 402.40
Triclinic, $P\overline{1}$
a = 9.4839 (18) Å
b = 10.3611 (19) Å
c = 11.276 (2) Å
α = 109.342 (3)°
β = 102.664 (3)°
γ = 97.985 (3)°
V = 992.8 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 (2) K
0.33 × 0.16 × 0.08 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.969, T_{max} = 0.992
5605 measured reflections
3819 independent reflections
2822 reflections with $I > 2\sigma(I)$
R_{int} = 0.013

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.119
S = 1.04
3819 reflections
271 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

*Cg*3 and *Cg*4 are the centroids of the C1–C6 and C10–C15 benzene rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3*B*···N3^{i}	0.93	2.48	3.328 (3)	151
C9—H9*B*···O1^{ii}	0.97	2.56	3.471 (2)	157
C15—H15*A*···O1^{ii}	0.93	2.46	3.368 (3)	164
C20—H20*A*···*Cg*3^{iii}	0.93	2.85	3.767	168
C22—H22*C*···*Cg*4^{iv}	0.96	2.87	3.530	127

Symmetry codes: (i) $-x+1, -y+2, -z+2$; (ii) $-x, -y+2, -z+1$; (iii) $x, y, z-1$; (iv) $x, y+1, z+1$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

This project was supported by the Natural Science Foundation of Shandong Province (grant No. Y2006B07).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2705).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Chen, Z.-Y. & Wu, M.-T. (2005). *Org. Lett.* **7**, 475–477.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Wan, J., Peng, Z.-Z., Li, X.-M. & Zhang, S.-S. (2006). *Acta Cryst.* E**62**, o634–o636.

supplementary materials

Acta Cryst. (2009). E**65**, o357 [**doi:10.1107/S1600536809001196**]

2-(1*H*-Benzotriazol-1-yl)-1-(3-methoxybenzoyl)ethyl isonicotinate

W. Wang and Z.-H. Mei

Comment

Benzotriazole and its derivatives exhibit an excellent pharmacological activities, such as antifungal, antitumor and antineoplastic activities (Chen & Wu, 2005). In order to find a new benzotriazole compound with higher bioactivity, the title compound, (I) (Fig. 1), was synthesized and its crystal structure was presented here.

In (I), all bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The benzotriazole ring is mostly planar with a dihedral angle of 1.75 (1)° between the N1—N3/C10/C11 triazole and C10—C15 benzene rings. The mean plane makes dihedral angles of 70.93 (1) and 19.8 (1)° with the N4/C17—C21 pyridine and C1—C6 benzene rings, respectively, and the dihedral angle between the latter two aromatic rings is 80.08 (1)°.

In the crystal structure, molecules of (I) are linked to each other by C3—H3B···N3, and further linked by C—H···O intermolecular hydrogen bonding interactions (C9—H9B···O1 and C15—H15A···O1), and stabilized by C—H···π interactions (Table 1). The distances of 3.783 Å between the centroids of the rings C10—C15 related by the symmetry code (-*x*, 1 - *y*, 1 - *z*) suggests a possible π–π interaction.

Experimental

The title compound was prepared according to the literature method of Wan *et al.* (20067). Single crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethyl acetate 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) and 1.5 U_{eq}(methyl C).

Figures

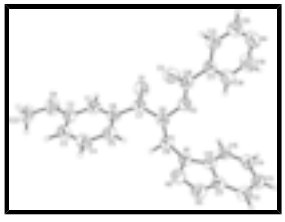


Fig. 1. The structure of the compound (I) showing 50% probability displacement ellipsoids and the atom numbering scheme.

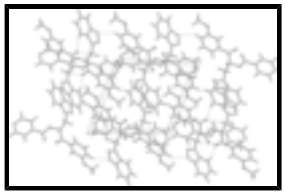


Fig. 2. A packing diagram of (I), viewed down the *a* axis. Hydrogen bonds are indicated by dashed lines.

2-(1*H*-Benzotriazol-1-yl)-1-(3-methoxybenzoyl)ethyl isonicotinate

Crystal data

$C_{22}H_{18}N_4O_4$	$Z = 2$
$M_r = 402.40$	$F_{000} = 420$
Triclinic, $P\overline{1}$	$D_x = 1.346$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.4839$ (18) Å	Cell parameters from 1711 reflections
$b = 10.3611$ (19) Å	$\theta = 2.6$–24.7°
$c = 11.276$ (2) Å	$\mu = 0.10$ mm^{-1}
$\alpha = 109.342$ (3)°	$T = 293$ (2) K
$\beta = 102.664$ (3)°	Plate, colourless
$\gamma = 97.985$ (3)°	0.33 × 0.16 × 0.08 mm
$V = 992.8$ (3) Å^3	

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	3819 independent reflections
Radiation source: fine-focus sealed tube	2822 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.013$
Detector resolution: 8.33 pixels mm^{-1}	$\theta_{max} = 26.1^\circ$
$T = 293(2)$ K	$\theta_{min} = 2.0^\circ$
ω scans	$h = -11 \rightarrow 11$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$k = -12 \rightarrow 10$
$T_{min} = 0.969$, $T_{max} = 0.992$	$l = -12 \rightarrow 13$
5605 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.046$	H-atom parameters constrained
$wR(F^2) = 0.119$	$w = 1/[\sigma^2(F_o^2) + (0.0502P)^2 + 0.1574P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$

3819 reflections	$\Delta\rho_{max} = 0.15$ e Å^{-3}
271 parameters	$\Delta\rho_{min} = -0.19$ 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 $F^2 > \sigma(F^2)$ 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}
O2	0.21549 (13)	0.94145 (12)	0.45684 (11)	0.0511 (3)
O3	0.40290 (15)	1.11047 (14)	0.47141 (13)	0.0639 (4)
N1	0.22089 (16)	0.73861 (15)	0.58935 (14)	0.0498 (4)
C7	0.23974 (18)	1.12532 (18)	0.66726 (18)	0.0474 (4)
C6	0.31816 (18)	1.19911 (18)	0.80934 (17)	0.0457 (4)
C17	0.23003 (19)	0.97219 (18)	0.26265 (17)	0.0481 (4)
C1	0.2728 (2)	1.31472 (19)	0.88006 (18)	0.0526 (5)
H1A	0.1952	1.3441	0.8379	0.063*
C16	0.29418 (19)	1.01773 (19)	0.40669 (18)	0.0487 (4)
O1	0.15281 (15)	1.17332 (14)	0.60783 (13)	0.0691 (4)
C8	0.26559 (19)	0.98062 (18)	0.59616 (17)	0.0474 (4)
H8A	0.3712	0.9811	0.6233	0.057*
N2	0.34386 (18)	0.72584 (18)	0.66902 (16)	0.0642 (5)
C10	0.16172 (19)	0.61663 (18)	0.48299 (17)	0.0457 (4)
C21	0.2851 (2)	1.0500 (2)	0.19695 (19)	0.0556 (5)
H21A	0.3604	1.1310	0.2422	0.067*
C9	0.1742 (2)	0.86971 (18)	0.62674 (18)	0.0498 (4)
H9A	0.1837	0.9040	0.7199	0.060*
H9B	0.0704	0.8535	0.5805	0.060*
C15	0.0363 (2)	0.57215 (19)	0.37579 (18)	0.0524 (5)
H15A	−0.0264	0.6310	0.3634	0.063*
N3	0.36612 (19)	0.60040 (18)	0.61744 (17)	0.0687 (5)
O4	0.28449 (18)	1.49647 (15)	1.07256 (15)	0.0812 (5)
C11	0.2550 (2)	0.52895 (19)	0.50226 (18)	0.0522 (5)
C5	0.4361 (2)	1.1570 (2)	0.87303 (19)	0.0565 (5)
H5A	0.4675	1.0791	0.8273	0.068*
C2	0.3411 (2)	1.38696 (19)	1.01200 (19)	0.0551 (5)
N4	0.1207 (2)	0.8890 (2)	−0.00867 (17)	0.0771 (5)

C3	0.4587 (2)	1.3456 (2)	1.0743 (2)	0.0626 (5)
H3B	0.5059	1.3944	1.1632	0.075*
C12	0.2266 (2)	0.3910 (2)	0.4131 (2)	0.0615 (5)
H12A	0.2887	0.3316	0.4253	0.074*
C14	0.0107 (2)	0.4364 (2)	0.28959 (19)	0.0604 (5)
H14A	−0.0717	0.4024	0.2164	0.072*
C4	0.5054 (2)	1.2319 (2)	1.0041 (2)	0.0670 (6)
H4B	0.5854	1.2052	1.0460	0.080*
C13	0.1044 (2)	0.3469 (2)	0.3078 (2)	0.0627 (5)
H13A	0.0826	0.2555	0.2466	0.075*
C20	0.2260 (2)	1.0049 (2)	0.0634 (2)	0.0680 (6)
H20A	0.2622	1.0593	0.0207	0.082*
C19	0.0693 (3)	0.8157 (3)	0.0559 (2)	0.0825 (7)
H19A	−0.0042	0.7339	0.0076	0.099*
C22	0.3532 (3)	1.5758 (2)	1.2089 (2)	0.0840 (7)
H22A	0.3031	1.6493	1.2391	0.126*
H22B	0.4555	1.6163	1.2223	0.126*
H22C	0.3471	1.5151	1.2570	0.126*
C18	0.1180 (2)	0.8531 (2)	0.1897 (2)	0.0695 (6)
H18A	0.0762	0.7991	0.2302	0.083*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0529 (7)	0.0520 (7)	0.0458 (7)	0.0072 (6)	0.0145 (6)	0.0166 (6)
O3	0.0558 (8)	0.0645 (9)	0.0632 (9)	−0.0020 (7)	0.0069 (7)	0.0265 (7)
N1	0.0547 (9)	0.0462 (9)	0.0449 (9)	0.0113 (7)	0.0066 (7)	0.0176 (7)
C7	0.0417 (9)	0.0488 (10)	0.0528 (11)	0.0117 (8)	0.0111 (8)	0.0213 (8)
C6	0.0435 (9)	0.0445 (10)	0.0490 (11)	0.0063 (8)	0.0119 (8)	0.0196 (8)
C17	0.0463 (10)	0.0511 (11)	0.0494 (11)	0.0166 (8)	0.0176 (8)	0.0172 (8)
C1	0.0477 (10)	0.0533 (11)	0.0565 (12)	0.0135 (8)	0.0109 (9)	0.0219 (9)
C16	0.0473 (10)	0.0476 (10)	0.0546 (11)	0.0149 (9)	0.0175 (9)	0.0199 (9)
O1	0.0717 (9)	0.0700 (9)	0.0587 (9)	0.0335 (8)	0.0025 (7)	0.0186 (7)
C8	0.0464 (10)	0.0486 (10)	0.0451 (10)	0.0114 (8)	0.0100 (8)	0.0165 (8)
N2	0.0651 (10)	0.0611 (11)	0.0550 (10)	0.0141 (8)	−0.0021 (8)	0.0197 (8)
C10	0.0511 (10)	0.0447 (10)	0.0426 (10)	0.0100 (8)	0.0128 (8)	0.0187 (8)
C21	0.0563 (11)	0.0538 (11)	0.0557 (12)	0.0126 (9)	0.0174 (9)	0.0185 (9)
C9	0.0546 (10)	0.0456 (10)	0.0479 (10)	0.0106 (8)	0.0146 (8)	0.0162 (8)
C15	0.0529 (11)	0.0565 (11)	0.0493 (11)	0.0154 (9)	0.0121 (9)	0.0221 (9)
N3	0.0723 (11)	0.0633 (11)	0.0633 (11)	0.0238 (9)	0.0017 (9)	0.0226 (9)
O4	0.0977 (11)	0.0704 (10)	0.0664 (10)	0.0311 (9)	0.0243 (9)	0.0088 (8)
C11	0.0577 (11)	0.0528 (11)	0.0476 (11)	0.0157 (9)	0.0101 (9)	0.0226 (9)
C5	0.0577 (11)	0.0552 (11)	0.0558 (12)	0.0196 (9)	0.0119 (9)	0.0196 (9)
C2	0.0593 (11)	0.0491 (11)	0.0535 (12)	0.0076 (9)	0.0178 (9)	0.0154 (9)
N4	0.0788 (12)	0.0912 (14)	0.0529 (11)	0.0082 (11)	0.0183 (10)	0.0213 (10)
C3	0.0667 (13)	0.0630 (13)	0.0483 (12)	0.0062 (10)	0.0070 (10)	0.0178 (10)
C12	0.0742 (13)	0.0531 (12)	0.0641 (13)	0.0248 (10)	0.0225 (11)	0.0245 (10)
C14	0.0603 (12)	0.0626 (13)	0.0485 (11)	0.0075 (10)	0.0118 (9)	0.0135 (9)

C4	0.0646 (13)	0.0745 (14)	0.0564 (13)	0.0205 (11)	0.0018 (10)	0.0258 (11)
C13	0.0761 (14)	0.0468 (11)	0.0595 (13)	0.0099 (10)	0.0231 (11)	0.0120 (9)
C20	0.0751 (14)	0.0726 (15)	0.0586 (13)	0.0117 (12)	0.0235 (11)	0.0266 (11)
C19	0.0799 (16)	0.0866 (17)	0.0563 (14)	−0.0113 (13)	0.0136 (12)	0.0116 (12)
C22	0.1063 (19)	0.0643 (14)	0.0660 (15)	0.0046 (13)	0.0360 (14)	0.0037 (11)
C18	0.0672 (13)	0.0733 (14)	0.0575 (13)	−0.0036 (11)	0.0170 (11)	0.0194 (11)

Geometric parameters (Å, °)

O2—C16	1.349 (2)	C15—H15A	0.9300
O2—C8	1.434 (2)	N3—C11	1.375 (2)
O3—C16	1.204 (2)	O4—C2	1.363 (2)
N1—N2	1.359 (2)	O4—C22	1.428 (2)
N1—C10	1.362 (2)	C11—C12	1.396 (3)
N1—C9	1.445 (2)	C5—C4	1.375 (3)
C7—O1	1.212 (2)	C5—H5A	0.9300
C7—C6	1.488 (2)	C2—C3	1.382 (3)
C7—C8	1.531 (2)	N4—C19	1.327 (3)
C6—C1	1.384 (2)	N4—C20	1.329 (3)
C6—C5	1.395 (2)	C3—C4	1.376 (3)
C17—C18	1.382 (3)	C3—H3B	0.9300
C17—C21	1.385 (3)	C12—C13	1.361 (3)
C17—C16	1.487 (2)	C12—H12A	0.9300
C1—C2	1.378 (3)	C14—C13	1.403 (3)
C1—H1A	0.9300	C14—H14A	0.9300
C8—C9	1.519 (2)	C4—H4B	0.9300
C8—H8A	0.9800	C13—H13A	0.9300
N2—N3	1.304 (2)	C20—H20A	0.9300
C10—C11	1.387 (2)	C19—C18	1.378 (3)
C10—C15	1.392 (2)	C19—H19A	0.9300
C21—C20	1.375 (3)	C22—H22A	0.9600
C21—H21A	0.9300	C22—H22B	0.9600
C9—H9A	0.9700	C22—H22C	0.9600
C9—H9B	0.9700	C18—H18A	0.9300
C15—C14	1.371 (3)		
C16—O2—C8	115.78 (13)	C2—O4—C22	117.93 (18)
N2—N1—C10	109.89 (14)	N3—C11—C10	108.94 (16)
N2—N1—C9	118.99 (14)	N3—C11—C12	130.21 (18)
C10—N1—C9	131.12 (15)	C10—C11—C12	120.83 (17)
O1—C7—C6	122.39 (16)	C4—C5—C6	119.33 (18)
O1—C7—C8	119.34 (16)	C4—C5—H5A	120.3
C6—C7—C8	118.21 (15)	C6—C5—H5A	120.3
C1—C6—C5	119.12 (17)	O4—C2—C1	115.94 (18)
C1—C6—C7	118.39 (15)	O4—C2—C3	124.37 (18)
C5—C6—C7	122.49 (16)	C1—C2—C3	119.69 (18)
C18—C17—C21	117.82 (18)	C19—N4—C20	116.16 (19)
C18—C17—C16	122.72 (18)	C4—C3—C2	119.54 (19)
C21—C17—C16	119.45 (17)	C4—C3—H3B	120.2
C2—C1—C6	120.96 (17)	C2—C3—H3B	120.2

C2—C1—H1A	119.5	C13—C12—C11	117.29 (18)
C6—C1—H1A	119.5	C13—C12—H12A	121.4
O3—C16—O2	123.70 (17)	C11—C12—H12A	121.4
O3—C16—C17	124.81 (18)	C15—C14—C13	122.40 (19)
O2—C16—C17	111.49 (15)	C15—C14—H14A	118.8
O2—C8—C9	106.06 (13)	C13—C14—H14A	118.8
O2—C8—C7	110.80 (14)	C5—C4—C3	121.34 (19)
C9—C8—C7	109.81 (14)	C5—C4—H4B	119.3
O2—C8—H8A	110.0	C3—C4—H4B	119.3
C9—C8—H8A	110.0	C12—C13—C14	121.34 (18)
C7—C8—H8A	110.0	C12—C13—H13A	119.3
N3—N2—N1	109.04 (15)	C14—C13—H13A	119.3
N1—C10—C11	104.25 (15)	N4—C20—C21	124.4 (2)
N1—C10—C15	133.49 (16)	N4—C20—H20A	117.8
C11—C10—C15	122.22 (16)	C21—C20—H20A	117.8
C20—C21—C17	118.61 (19)	N4—C19—C18	124.2 (2)
C20—C21—H21A	120.7	N4—C19—H19A	117.9
C17—C21—H21A	120.7	C18—C19—H19A	117.9
N1—C9—C8	111.93 (14)	O4—C22—H22A	109.5
N1—C9—H9A	109.2	O4—C22—H22B	109.5
C8—C9—H9A	109.2	H22A—C22—H22B	109.5
N1—C9—H9B	109.2	O4—C22—H22C	109.5
C8—C9—H9B	109.2	H22A—C22—H22C	109.5
H9A—C9—H9B	107.9	H22B—C22—H22C	109.5
C14—C15—C10	115.92 (17)	C19—C18—C17	118.8 (2)
C14—C15—H15A	122.0	C19—C18—H18A	120.6
C10—C15—H15A	122.0	C17—C18—H18A	120.6
N2—N3—C11	107.87 (15)		

O1—C7—C6—C1	10.4 (3)	N1—C10—C15—C14	−177.61 (19)
C8—C7—C6—C1	−166.80 (16)	C11—C10—C15—C14	−0.4 (3)
O1—C7—C6—C5	−168.84 (18)	N1—N2—N3—C11	−0.5 (2)
C8—C7—C6—C5	13.9 (3)	N2—N3—C11—C10	0.6 (2)
C5—C6—C1—C2	−0.9 (3)	N2—N3—C11—C12	−177.9 (2)
C7—C6—C1—C2	179.82 (17)	N1—C10—C11—N3	−0.4 (2)
C8—O2—C16—O3	2.3 (2)	C15—C10—C11—N3	−178.31 (17)
C8—O2—C16—C17	−177.93 (13)	N1—C10—C11—C12	178.28 (18)
C18—C17—C16—O3	170.73 (19)	C15—C10—C11—C12	0.4 (3)
C21—C17—C16—O3	−8.3 (3)	C1—C6—C5—C4	−0.6 (3)
C18—C17—C16—O2	−9.0 (2)	C7—C6—C5—C4	178.69 (18)
C21—C17—C16—O2	172.00 (15)	C22—O4—C2—C1	−179.05 (18)
C16—O2—C8—C9	−172.79 (13)	C22—O4—C2—C3	1.4 (3)
C16—O2—C8—C7	68.10 (18)	C6—C1—C2—O4	−178.11 (17)
O1—C7—C8—O2	18.0 (2)	C6—C1—C2—C3	1.5 (3)
C6—C7—C8—O2	−164.64 (14)	O4—C2—C3—C4	178.9 (2)
O1—C7—C8—C9	−98.8 (2)	C1—C2—C3—C4	−0.6 (3)
C6—C7—C8—C9	78.53 (19)	N3—C11—C12—C13	178.3 (2)
C10—N1—N2—N3	0.3 (2)	C10—C11—C12—C13	−0.1 (3)
C9—N1—N2—N3	−179.98 (16)	C10—C15—C14—C13	0.2 (3)
N2—N1—C10—C11	0.1 (2)	C6—C5—C4—C3	1.5 (3)

C9—N1—C10—C11	−179.61 (17)	C2—C3—C4—C5	−0.9 (3)
N2—N1—C10—C15	177.64 (19)	C11—C12—C13—C14	−0.1 (3)
C9—N1—C10—C15	−2.1 (3)	C15—C14—C13—C12	0.0 (3)
C18—C17—C21—C20	−0.1 (3)	C19—N4—C20—C21	1.4 (3)
C16—C17—C21—C20	178.95 (17)	C17—C21—C20—N4	−1.5 (3)
N2—N1—C9—C8	79.2 (2)	C20—N4—C19—C18	0.2 (4)
C10—N1—C9—C8	−101.1 (2)	N4—C19—C18—C17	−1.7 (4)
O2—C8—C9—N1	74.36 (17)	C21—C17—C18—C19	1.6 (3)
C7—C8—C9—N1	−165.87 (14)	C16—C17—C18—C19	−177.42 (19)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3B···N3^{i}	0.93	2.48	3.328 (3)	151
C9—H9B···O1^{ii}	0.97	2.56	3.471 (2)	157
C15—H15A···O1^{ii}	0.93	2.46	3.368 (3)	164
C20—H20A···Cg3^{iii}	0.93	2.85	3.767	168
C22—H22C···Cg4^{iv}	0.96	2.87	3.530	127

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

Fig. 1

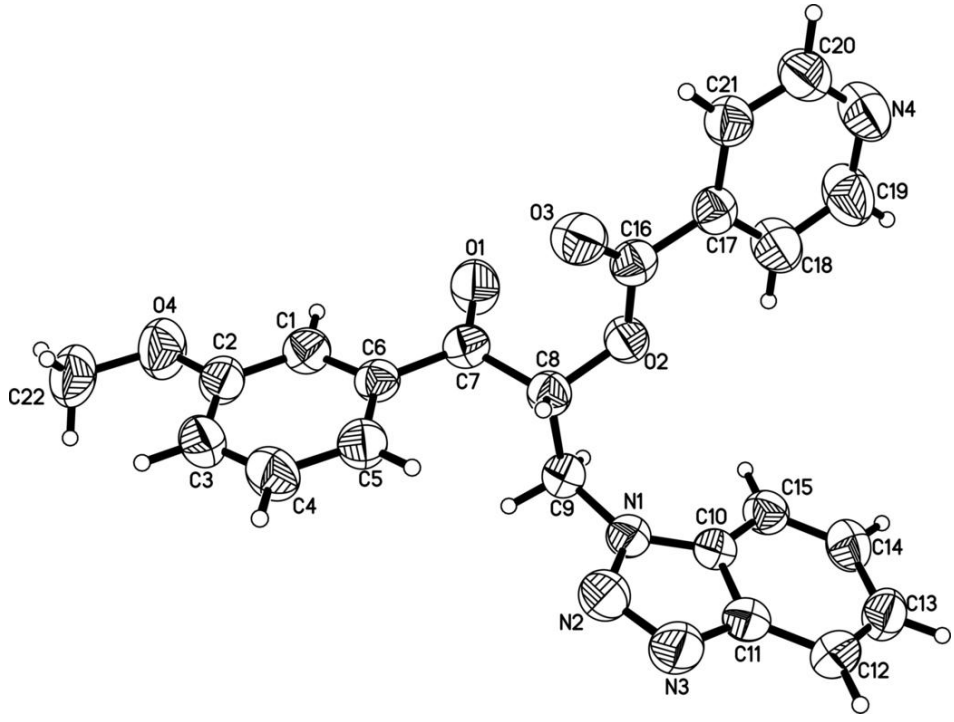

C20
C21
N4
C19
O3
C16
C17
C18
O1
O4
C1
C2
C6
C7
C8
O2
C22
C3
C4
C5
C9
N1
C10
C15
C14
C13
N2
C11
C12
N3

Fig. 2