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2-(1*H*-Benzotriazol-1-yl)-1-(3-bromobenzoyl)ethyl benzoate. Corrigendum

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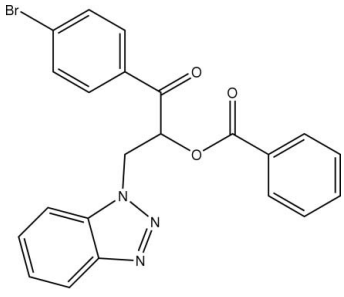
The chemical name of the title compound in the paper by Hu & Wang [*Acta Cryst.* (2009), E**65**, o392] is corrected and the structural diagram is updated.

In the paper by Hu & Wang [*Acta Cryst.* (2009), E**65**, o392], the chemical name given in the *Title* should be '2-(1*H*-Benzotriazol-1-yl)-1-(4-bromobenzoyl)ethyl benzoate'. An updated structural diagram is shown below.



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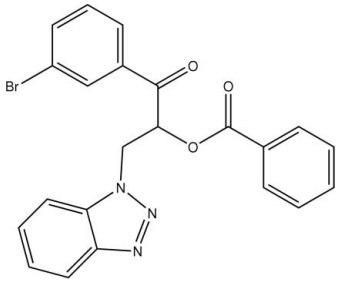
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.040; wR factor = 0.101; data-to-parameter ratio = 14.4.

In the title compound, $C_{22}H_{16}BrN_3O_3$, the dihedral angles between the benzotriazole mean plane and the benzene rings of 4.84 (1) and 89.50 (1)°. The dihedral angle between the two benzene rings is 84.77 (1)°. In the crystal structure, molecules are linked into chains by intermolecular C—H···O hydrogen bonds. The crystal packing is further stabilized by C—H···π interactions.

Related literature

For general background on benzotriazoles, see: Xu *et al.* (2003). For the synthesis, see: Zhang *et al.* (2006). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{22}H_{16}BrN_3O_3$
M_r = 450.28
Triclinic, $P\overline{1}$
a = 6.4390 (12) Å
b = 8.8267 (17) Å
c = 17.430 (3) Å
α = 88.589 (3)°
β = 85.024 (3)°
γ = 83.087 (3)°
V = 979.6 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.13 mm^{-1}
T = 293 (2) K
0.42 × 0.12 × 0.10 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.469, T_{max} = 0.815
5526 measured reflections
3773 independent reflections
2885 reflections with $I > 2\sigma(I)$
R_{int} = 0.015

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.101
S = 1.04
3773 reflections
262 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

*Cg*1 is the centroid of the N1–N3/C17/C18 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16A···*Cg*1^{i}	0.93	2.78	3.571	144
C21—H21A···O3^{ii}	0.93	2.47	3.202 (4)	136

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

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 Nos. Y2008B02 and Y2008B32).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2710).

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Zhang, S.-S., Wan, J., Peng, Z.-Z. & Bi, S. (2006). *Acta Cryst.* E**62**, o4348–o4349.

supporting information

Acta Cryst. (2009). E**65**, o392 [doi:10.1107/S1600536809002608]

2-(1*H*-Benzotriazol-1-yl)-1-(3-bromobenzoyl)ethyl benzoate

Kong-Cheng Hu and Wei Wang

S1. Comment

Benzotriazole derivatives have become the most efficient antifungal compounds with the properties of low toxicity, high oral bioavailability and so on (Xu *et al.*, 2003). In order to search for new benzotriazole compounds with higher bioactivity, the title compound, (I), was synthesized, and its structure is presented here.

In the title compound (I) (Fig. 1), all bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The benzotriazole ring is essentially planar with a dihedral angle of 0.29 (15)°. The whole molecule is non-planar, with the dihedral angles between the benzotriazole mean plane and C1–C6 and C11–C16 benzene rings of 4.84 (1) and 89.50 (1)°, respectively. The dihedral angle between the two benzene rings is 84.77 (1)°.

In the crystal structure (Fig. 2), molecules are linked into chains along *b* axis by C21—H21A···O3 intermolecular hydrogen bonds (Table 1). Furthermore, the crystal packing is further stabilized by C—H···π interactions (Table 1).

S2. Experimental

The title compound was prepared according to the literature method of Zhang *et al.* (2006). Single crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethyl acetate solution at room temperature over a period of six days.

S3. 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 0.93–0.978 Å, and with U_{iso}(H) = 1.2 U_{eq}(C).

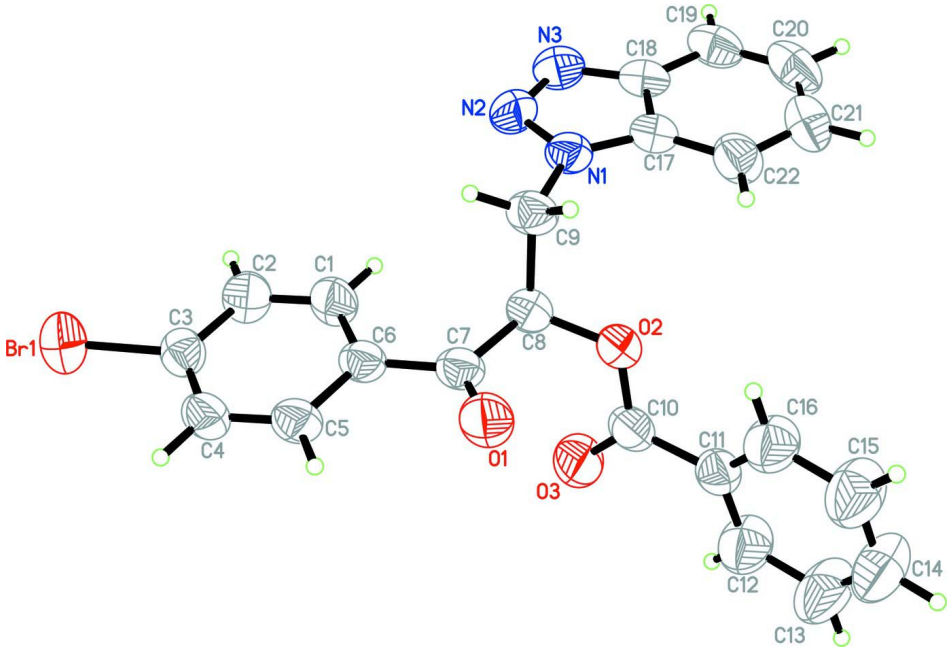

Figure 1

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

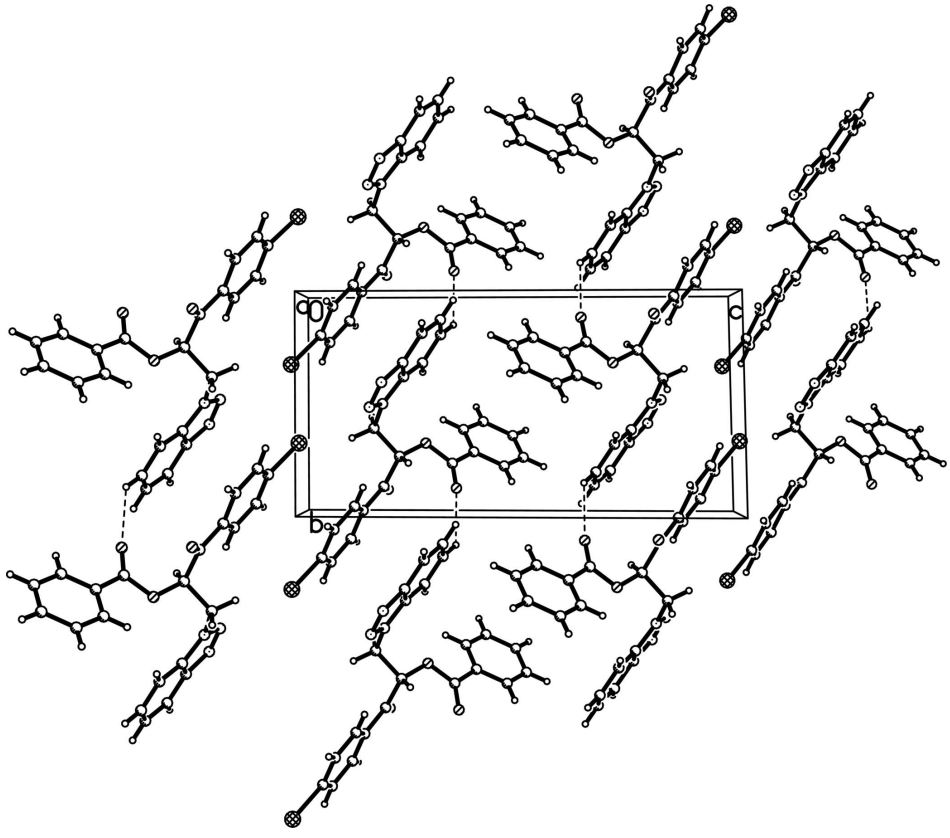

Figure 2

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-bromobenzoyl)ethyl benzoate

Crystal data

$C_{22}H_{16}BrN_3O_3$
$M_r = 450.28$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.4390$ (12) Å
$b = 8.8267$ (17) Å
$c = 17.430$ (3) Å
$\alpha = 88.589$ (3)°
$\beta = 85.024$ (3)°
$\gamma = 83.087$ (3)°
$V = 979.6$ (3) Å^3
$Z = 2$
$F(000) = 456$
$D_x = 1.527$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2027 reflections
$\theta = 2.3$–$24.1°$
$\mu = 2.13$ mm^{-1}
$T = 293$ K
Column, colourless
0.42 × 0.12 × 0.10 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.33 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.469$, $T_{max} = 0.815$
5526 measured reflections
3773 independent reflections
2885 reflections with $I > 2\sigma(I)$
$R_{int} = 0.015$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.3°$
$h = -5 \rightarrow 7$
$k = -8 \rightarrow 10$
$l = -21 \rightarrow 21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.101$
$S = 1.04$
3773 reflections
262 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0529P)^2 + 0.1162P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.45$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}

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}
Br1	0.15134 (5)	0.67410 (4)	0.013609 (18)	0.07266 (15)
O1	0.8295 (3)	1.1006 (2)	−0.19239 (12)	0.0665 (5)
O2	0.6637 (3)	1.31723 (18)	−0.28399 (10)	0.0539 (5)

N2	0.0957 (4)	1.4833 (3)	−0.16528 (13)	0.0589 (6)
N1	0.2970 (3)	1.4981 (2)	−0.19112 (12)	0.0493 (5)
C3	0.2999 (4)	0.8086 (3)	−0.04996 (15)	0.0516 (6)
O3	0.6428 (4)	1.1121 (2)	−0.35433 (12)	0.0761 (6)
C17	0.3044 (4)	1.6208 (3)	−0.23960 (14)	0.0471 (6)
C7	0.6396 (4)	1.1190 (3)	−0.18590 (15)	0.0490 (6)
C4	0.5140 (4)	0.7794 (3)	−0.06486 (15)	0.0557 (7)
H4A	0.5862	0.6915	−0.0451	0.067*
C6	0.5140 (4)	1.0130 (3)	−0.13989 (14)	0.0471 (6)
C8	0.5243 (4)	1.2583 (3)	−0.22507 (15)	0.0499 (6)
H8A	0.3993	1.2305	−0.2470	0.060*
C2	0.1912 (4)	0.9376 (3)	−0.08071 (16)	0.0582 (7)
H2B	0.0461	0.9562	−0.0710	0.070*
C10	0.7238 (4)	1.2242 (3)	−0.34460 (15)	0.0544 (7)
C5	0.6206 (4)	0.8806 (3)	−0.10897 (15)	0.0535 (6)
H5A	0.7656	0.8612	−0.1185	0.064*
C18	0.0959 (4)	1.6813 (3)	−0.24132 (15)	0.0511 (6)
N3	−0.0275 (4)	1.5931 (3)	−0.19522 (14)	0.0624 (6)
C1	0.2975 (4)	1.0380 (3)	−0.12556 (16)	0.0560 (7)
H1A	0.2235	1.1238	−0.1466	0.067*
C9	0.4638 (4)	1.3866 (3)	−0.16730 (15)	0.0541 (6)
H9A	0.4194	1.3430	−0.1178	0.065*
H9B	0.5863	1.4376	−0.1608	0.065*
C22	0.4686 (5)	1.6847 (3)	−0.28088 (18)	0.0610 (7)
H22A	0.6080	1.6432	−0.2793	0.073*
C11	0.9024 (4)	1.2743 (3)	−0.39390 (15)	0.0535 (6)
C21	0.4115 (5)	1.8121 (3)	−0.3239 (2)	0.0726 (9)
H21A	0.5153	1.8587	−0.3526	0.087*
C19	0.0423 (5)	1.8118 (3)	−0.28590 (18)	0.0631 (8)
H19A	−0.0968	1.8536	−0.2879	0.076*
C12	0.9535 (6)	1.2079 (4)	−0.46490 (18)	0.0778 (9)
H12A	0.8719	1.1376	−0.4820	0.093*
C16	1.0265 (5)	1.3774 (4)	−0.36929 (18)	0.0721 (9)
H16A	0.9933	1.4227	−0.3215	0.086*
C20	0.2004 (6)	1.8749 (3)	−0.32606 (19)	0.0748 (9)
H20A	0.1688	1.9621	−0.3559	0.090*
C14	1.2476 (6)	1.3470 (5)	−0.4857 (2)	0.0931 (11)
H14A	1.3641	1.3710	−0.5169	0.112*
C15	1.1998 (6)	1.4135 (5)	−0.4154 (2)	0.0915 (11)
H15A	1.2835	1.4827	−0.3986	0.110*
C13	1.1247 (6)	1.2457 (5)	−0.5102 (2)	0.0958 (12)
H13A	1.1575	1.2017	−0.5583	0.115*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0764 (3)	0.0699 (2)	0.0733 (2)	−0.01787 (16)	−0.00824 (16)	0.01757 (16)
O1	0.0458 (12)	0.0633 (12)	0.0861 (14)	0.0045 (9)	−0.0008 (10)	0.0130 (10)

O2	0.0662 (12)	0.0404 (9)	0.0529 (11)	−0.0038 (8)	0.0035 (9)	−0.0007 (8)
N2	0.0512 (14)	0.0594 (14)	0.0609 (14)	0.0033 (11)	0.0100 (11)	0.0006 (11)
N1	0.0467 (12)	0.0456 (12)	0.0524 (12)	0.0060 (9)	−0.0012 (10)	−0.0012 (9)
C3	0.0587 (17)	0.0502 (15)	0.0470 (14)	−0.0080 (12)	−0.0096 (12)	0.0009 (11)
O3	0.1015 (17)	0.0571 (12)	0.0724 (14)	−0.0305 (12)	0.0110 (12)	−0.0155 (10)
C17	0.0480 (15)	0.0415 (13)	0.0508 (14)	0.0003 (11)	−0.0052 (11)	−0.0084 (11)
C7	0.0484 (16)	0.0452 (14)	0.0505 (15)	0.0058 (11)	−0.0038 (12)	−0.0022 (11)
C4	0.0607 (18)	0.0470 (15)	0.0564 (16)	0.0070 (12)	−0.0089 (13)	0.0052 (12)
C6	0.0468 (15)	0.0446 (14)	0.0477 (14)	0.0042 (11)	−0.0048 (11)	−0.0015 (11)
C8	0.0499 (15)	0.0448 (14)	0.0533 (15)	0.0007 (11)	−0.0031 (12)	0.0011 (11)
C2	0.0429 (15)	0.0668 (18)	0.0640 (17)	−0.0027 (13)	−0.0073 (13)	0.0078 (14)
C10	0.0697 (18)	0.0393 (14)	0.0529 (16)	−0.0020 (13)	−0.0046 (13)	−0.0002 (12)
C5	0.0464 (15)	0.0509 (15)	0.0597 (16)	0.0084 (12)	−0.0055 (12)	0.0009 (12)
C18	0.0504 (16)	0.0462 (14)	0.0551 (16)	0.0057 (12)	−0.0070 (12)	−0.0133 (12)
N3	0.0502 (14)	0.0616 (15)	0.0707 (16)	0.0059 (11)	0.0052 (12)	−0.0054 (12)
C1	0.0476 (16)	0.0549 (16)	0.0633 (17)	0.0046 (12)	−0.0095 (13)	0.0093 (13)
C9	0.0585 (16)	0.0489 (15)	0.0519 (15)	0.0098 (12)	−0.0093 (12)	−0.0006 (12)
C22	0.0541 (17)	0.0493 (16)	0.080 (2)	−0.0081 (13)	−0.0049 (14)	−0.0004 (14)
C11	0.0685 (18)	0.0447 (14)	0.0460 (14)	−0.0036 (12)	−0.0016 (12)	0.0014 (11)
C21	0.084 (2)	0.0511 (17)	0.085 (2)	−0.0206 (16)	−0.0047 (18)	0.0065 (15)
C19	0.0685 (19)	0.0480 (16)	0.0713 (19)	0.0103 (14)	−0.0190 (15)	−0.0072 (14)
C12	0.095 (2)	0.083 (2)	0.0592 (19)	−0.0282 (19)	0.0034 (17)	−0.0146 (17)
C16	0.083 (2)	0.075 (2)	0.0601 (18)	−0.0211 (17)	0.0040 (16)	−0.0129 (15)
C20	0.103 (3)	0.0417 (16)	0.081 (2)	0.0013 (16)	−0.0285 (19)	0.0060 (15)
C14	0.088 (3)	0.121 (3)	0.072 (2)	−0.034 (2)	0.017 (2)	−0.006 (2)
C15	0.093 (3)	0.105 (3)	0.082 (2)	−0.043 (2)	0.009 (2)	−0.017 (2)
C13	0.109 (3)	0.120 (3)	0.059 (2)	−0.035 (3)	0.021 (2)	−0.020 (2)

Geometric parameters (Å, º)

Br1—C3	1.891 (3)	C5—H5A	0.9300
O1—C7	1.210 (3)	C18—N3	1.375 (4)
O2—C10	1.355 (3)	C18—C19	1.399 (4)
O2—C8	1.435 (3)	C1—H1A	0.9300
N2—N3	1.305 (3)	C9—H9A	0.9700
N2—N1	1.355 (3)	C9—H9B	0.9700
N1—C17	1.360 (3)	C22—C21	1.367 (4)
N1—C9	1.448 (3)	C22—H22A	0.9300
C3—C4	1.374 (4)	C11—C12	1.379 (4)
C3—C2	1.385 (4)	C11—C16	1.380 (4)
O3—C10	1.195 (3)	C21—C20	1.409 (5)
C17—C18	1.386 (4)	C21—H21A	0.9300
C17—C22	1.394 (4)	C19—C20	1.353 (4)
C7—C6	1.485 (4)	C19—H19A	0.9300
C7—C8	1.535 (3)	C12—C13	1.369 (5)
C4—C5	1.372 (4)	C12—H12A	0.9300
C4—H4A	0.9300	C16—C15	1.382 (4)
C6—C1	1.387 (4)	C16—H16A	0.9300

C6—C5	1.402 (3)	C20—H20A	0.9300
C8—C9	1.527 (4)	C14—C13	1.362 (5)
C8—H8A	0.9800	C14—C15	1.368 (5)
C2—C1	1.373 (4)	C14—H14A	0.9300
C2—H2B	0.9300	C15—H15A	0.9300
C10—C11	1.480 (4)	C13—H13A	0.9300

C10—O2—C8	115.31 (19)	C2—C1—C6	120.8 (2)
N3—N2—N1	108.8 (2)	C2—C1—H1A	119.6
N2—N1—C17	110.4 (2)	C6—C1—H1A	119.6
N2—N1—C9	119.2 (2)	N1—C9—C8	112.8 (2)
C17—N1—C9	130.4 (2)	N1—C9—H9A	109.0
C4—C3—C2	120.3 (2)	C8—C9—H9A	109.0
C4—C3—Br1	120.3 (2)	N1—C9—H9B	109.0
C2—C3—Br1	119.3 (2)	C8—C9—H9B	109.0
N1—C17—C18	103.9 (2)	H9A—C9—H9B	107.8
N1—C17—C22	133.2 (2)	C21—C22—C17	115.7 (3)
C18—C17—C22	122.9 (2)	C21—C22—H22A	122.1
O1—C7—C6	122.2 (2)	C17—C22—H22A	122.1
O1—C7—C8	119.0 (2)	C12—C11—C16	119.2 (3)
C6—C7—C8	118.8 (2)	C12—C11—C10	118.4 (3)
C5—C4—C3	119.7 (2)	C16—C11—C10	122.3 (2)
C5—C4—H4A	120.1	C22—C21—C20	122.1 (3)
C3—C4—H4A	120.1	C22—C21—H21A	119.0
C1—C6—C5	118.3 (2)	C20—C21—H21A	119.0
C1—C6—C7	123.6 (2)	C20—C19—C18	117.5 (3)
C5—C6—C7	118.1 (2)	C20—C19—H19A	121.2
O2—C8—C9	105.9 (2)	C18—C19—H19A	121.2
O2—C8—C7	109.4 (2)	C13—C12—C11	119.9 (3)
C9—C8—C7	110.1 (2)	C13—C12—H12A	120.1
O2—C8—H8A	110.4	C11—C12—H12A	120.1
C9—C8—H8A	110.4	C11—C16—C15	120.3 (3)
C7—C8—H8A	110.4	C11—C16—H16A	119.9
C1—C2—C3	120.0 (2)	C15—C16—H16A	119.9
C1—C2—H2B	120.0	C19—C20—C21	121.7 (3)
C3—C2—H2B	120.0	C19—C20—H20A	119.1
O3—C10—O2	122.4 (2)	C21—C20—H20A	119.1
O3—C10—C11	125.0 (2)	C13—C14—C15	120.0 (3)
O2—C10—C11	112.5 (2)	C13—C14—H14A	120.0
C4—C5—C6	121.0 (2)	C15—C14—H14A	120.0
C4—C5—H5A	119.5	C14—C15—C16	119.7 (3)
C6—C5—H5A	119.5	C14—C15—H15A	120.1
N3—C18—C17	109.1 (2)	C16—C15—H15A	120.1
N3—C18—C19	130.8 (3)	C14—C13—C12	120.9 (3)
C17—C18—C19	120.1 (3)	C14—C13—H13A	119.5
N2—N3—C18	107.9 (2)	C12—C13—H13A	119.5

N3—N2—N1—C17	−0.3 (3)	N1—N2—N3—C18	−0.2 (3)

N3—N2—N1—C9	−178.5 (2)	C17—C18—N3—N2	0.5 (3)
N2—N1—C17—C18	0.6 (3)	C19—C18—N3—N2	−179.8 (3)
C9—N1—C17—C18	178.5 (2)	C3—C2—C1—C6	−0.8 (4)
N2—N1—C17—C22	−180.0 (3)	C5—C6—C1—C2	1.6 (4)
C9—N1—C17—C22	−2.0 (5)	C7—C6—C1—C2	−178.1 (3)
C2—C3—C4—C5	1.5 (4)	N2—N1—C9—C8	94.5 (3)
Br1—C3—C4—C5	−177.8 (2)	C17—N1—C9—C8	−83.3 (3)
O1—C7—C6—C1	174.0 (3)	O2—C8—C9—N1	81.7 (3)
C8—C7—C6—C1	−4.7 (4)	C7—C8—C9—N1	−160.1 (2)
O1—C7—C6—C5	−5.7 (4)	N1—C17—C22—C21	−179.5 (3)
C8—C7—C6—C5	175.6 (2)	C18—C17—C22—C21	−0.1 (4)
C10—O2—C8—C9	−175.1 (2)	O3—C10—C11—C12	14.4 (4)
C10—O2—C8—C7	66.3 (3)	O2—C10—C11—C12	−167.9 (3)
O1—C7—C8—O2	18.8 (3)	O3—C10—C11—C16	−161.4 (3)
C6—C7—C8—O2	−162.4 (2)	O2—C10—C11—C16	16.3 (4)
O1—C7—C8—C9	−97.1 (3)	C17—C22—C21—C20	0.2 (5)
C6—C7—C8—C9	81.6 (3)	N3—C18—C19—C20	−179.9 (3)
C4—C3—C2—C1	−0.8 (4)	C17—C18—C19—C20	−0.3 (4)
Br1—C3—C2—C1	178.6 (2)	C16—C11—C12—C13	−0.5 (5)
C8—O2—C10—O3	10.9 (4)	C10—C11—C12—C13	−176.5 (3)
C8—O2—C10—C11	−166.9 (2)	C12—C11—C16—C15	0.0 (5)
C3—C4—C5—C6	−0.7 (4)	C10—C11—C16—C15	175.8 (3)
C1—C6—C5—C4	−0.8 (4)	C18—C19—C20—C21	0.4 (5)
C7—C6—C5—C4	178.9 (2)	C22—C21—C20—C19	−0.4 (5)
N1—C17—C18—N3	−0.7 (3)	C13—C14—C15—C16	0.0 (7)
C22—C17—C18—N3	179.8 (2)	C11—C16—C15—C14	0.3 (6)
N1—C17—C18—C19	179.6 (2)	C15—C14—C13—C12	−0.5 (7)
C22—C17—C18—C19	0.1 (4)	C11—C12—C13—C14	0.8 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16*A*···*Cg*1^{i}	0.93	2.78	3.571	144
C21—H21*A*···O3^{ii}	0.93	2.47	3.202 (4)	136

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