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2-(1*H*-Benzotriazol-1-yl)-1-(4-bromobenzoyl)ethyl 4-methylbenzoate

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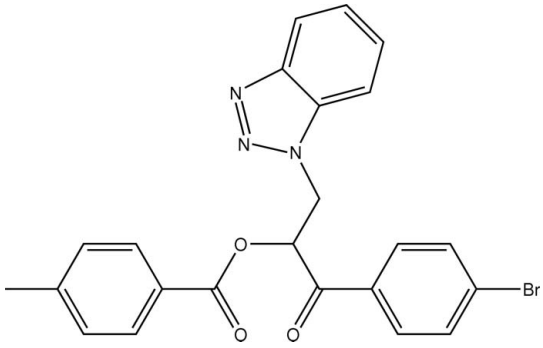
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.041; wR factor = 0.100; data-to-parameter ratio = 14.1.

In the molecule of the title compound, $C_{23}H_{18}BrN_3O_3$, the benzotriazole mean plane makes dihedral angles of 1.26 (1) and 87.39 (1)° with the tolyl and bromophenyl benzene rings, respectively, and the dihedral angle between the benzene rings is 87.27 (1)°. In the crystal structure, molecules are linked into chains along the a axis by C—H···O intermolecular hydrogen bonds. The structure is further stabilized by C—H···π and π–π interactions, with a distance of 3.700 (1) Å between the centroids of the bromophenyl and benzotriazole benzene rings related by symmetry code (x, $-1+y$, z).

Related literature

For related literature, see: Wan *et al.* (2006). For reference structural data, see Allen *et al.*, (1987).



Experimental

Crystal data

$C_{23}H_{18}BrN_3O_3$
M_r = 464.30
Triclinic, $P\overline{1}$
a = 6.995 (2) Å
b = 9.038 (2) Å
c = 16.909 (5) Å
α = 87.617 (5)°
β = 85.741 (5)°
γ = 74.688 (5)°
V = 1027.8 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.03 mm^{-1}
T = 293 (2) K
0.35 × 0.12 × 0.07 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.537, T_{max} = 0.871
5629 measured reflections
3814 independent reflections
2852 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.100
S = 1.01
3814 reflections
271 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 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
C15—H15A···$Cg1^{i}$	0.93	2.86	3.596 (1)	138
C2—H2A···O1^{ii}	0.93	2.56	3.292 (4)	137

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2508).

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supporting information

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2-(1*H*-Benzotriazol-1-yl)-1-(4-bromobenzoyl)ethyl 4-methylbenzoate

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S1. Comment

Recently, we have reported the structure of 2-(1*H*-1,2,3-benzotriazol-1-ylmethyl)-1-benzoylethyl 4-chlorobenzoate (II) (Wan *et al.*, 2006). As part of our ongoing studies on new benzotriazole derivatives with higher bioactivity, the title compound, (I), was synthesized and its structure is presented here.

In the molecule of (I), all bond lengths and angles are within normal ranges (Allen *et al.*, 1987) and are comparable with those in the related compound, (II). The benzotriazole system is essentially planar with a dihedral angle of 1.14 (2)° between the N1–N3/C17/C18 triazole ring and C17–C22 benzene ring. The benzotriazole mean plane makes dihedral angles of 1.26 (1)° and 87.39 (1)°, respectively, with the two benzene rings C1–C6 and C11–C16. The dihedral angle between the benzene rings is 87.27 (1)°.

In the crystal structure (Fig. 2), intermolecular C1—H2A···O1 hydrogen bonds (Table 1) link the molecules into infinite chains along the *a* axis. The molecules are further stabilized by C—H···π interactions (Table 1). The distance of 3.700 (1) Å between the centroids of benzene rings C1–C6 and C17–C22 related by symmetry code (x, -1 + y, z) suggests a possible π–π interactions.

S2. Experimental

The title compound was prepared according to the literature method of Wan *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 a week.

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 0.93–0.97 Å, and with U_{iso}(H) = 1.2 or 1.5 U_{eq}(C) H atoms.

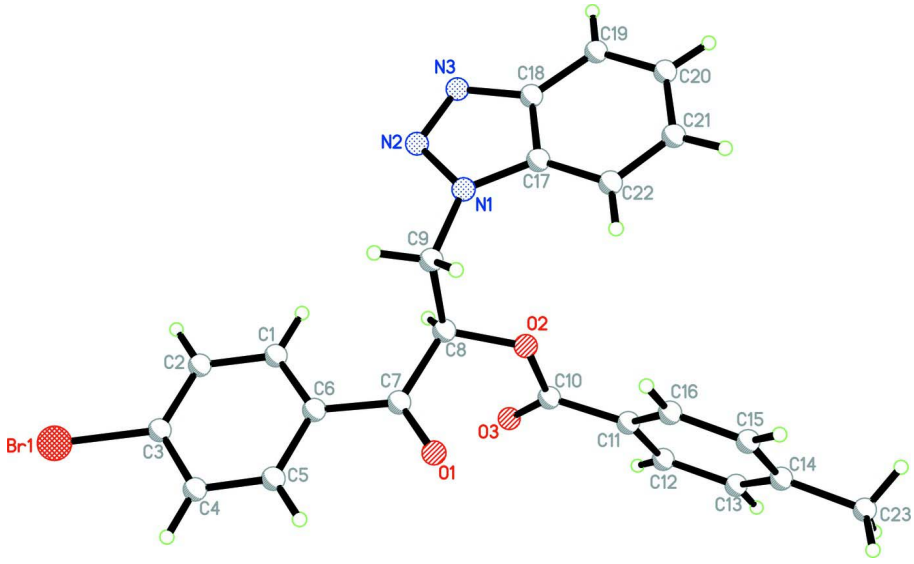

Figure 1

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

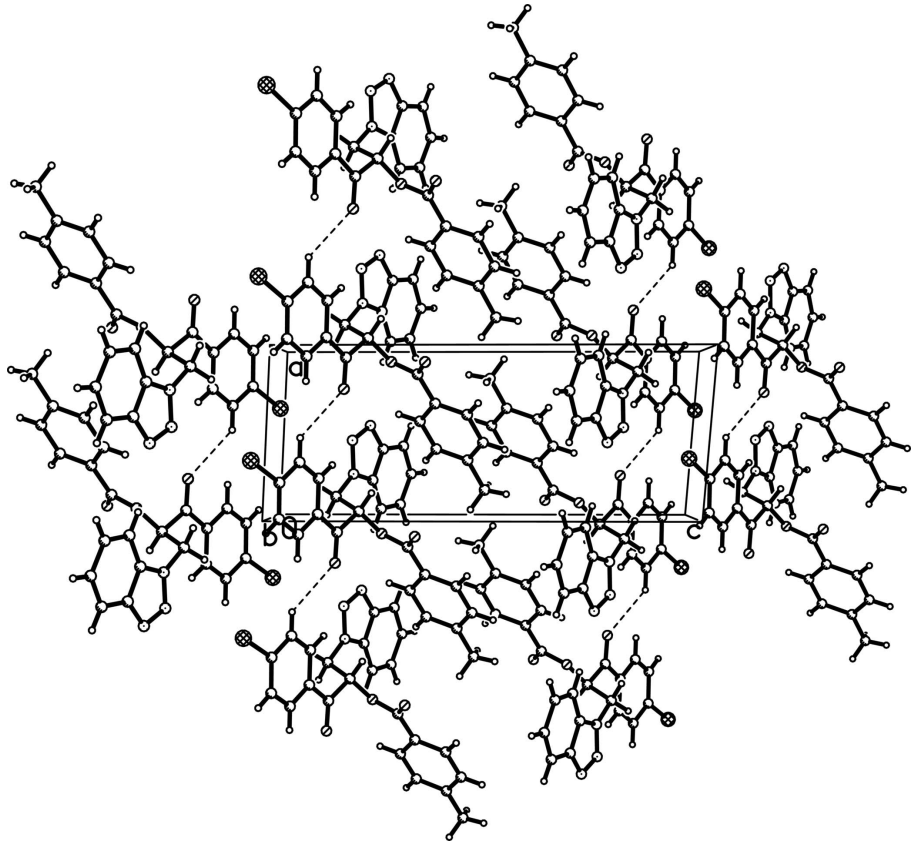

Figure 2

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

2-(1*H*-Benzotriazol-1-yl)-1-(4-bromobenzoyl)ethyl 4-methylbenzoate

Crystal data

$C_{23}H_{18}BrN_3O_3$
$M_r = 464.30$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.995$ (2) Å
$b = 9.038$ (2) Å
$c = 16.909$ (5) Å
$\alpha = 87.617$ (5)°
$\beta = 85.741$ (5)°
$\gamma = 74.688$ (5)°
$V = 1027.8$ (5) Å^3
$Z = 2$
$F(000) = 472$
$D_x = 1.500$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1830 reflections
$\theta = 2.4$–22.9°
$\mu = 2.03$ mm^{-1}
$T = 293$ K
Block, colourless
0.35 × 0.12 × 0.07 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)
$T_{min} = 0.537$, $T_{max} = 0.871$
5629 measured reflections
3814 independent reflections
2852 reflections with $I > 2\sigma(I)$
$R_{int} = 0.016$
$\theta_{max} = 25.7°$, $\theta_{min} = 2.3°$
$h = -8\rightarrow7$
$k = -11\rightarrow11$
$l = -20\rightarrow16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.100$
$S = 1.01$
3814 reflections
271 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
$w = 1/[\sigma^2(F_o^2) + (0.0475P)^2 + 0.3285P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.40$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ 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	0.64770 (5)	0.65794 (4)	0.01583 (2)	0.06665 (16)
O2	1.0846 (3)	1.2940 (2)	−0.26852 (11)	0.0472 (5)
N1	0.7376 (3)	1.5016 (3)	−0.18983 (14)	0.0455 (6)

O3	1.0928 (3)	1.1006 (2)	−0.34871 (13)	0.0603 (6)
O1	1.2452 (3)	1.0717 (3)	−0.16910 (15)	0.0699 (7)
C2	0.6600 (4)	0.9193 (3)	−0.08211 (18)	0.0488 (7)
H2A	0.5225	0.9380	−0.0802	0.059*
C3	0.7730 (4)	0.7930 (3)	−0.04374 (17)	0.0453 (7)
C7	1.0667 (4)	1.0962 (3)	−0.16942 (17)	0.0470 (7)
C6	0.9582 (4)	0.9930 (3)	−0.12617 (16)	0.0415 (7)
C17	0.7777 (4)	1.6225 (3)	−0.23346 (17)	0.0413 (7)
C10	1.1583 (4)	1.2049 (3)	−0.33201 (17)	0.0445 (7)
C4	0.9777 (4)	0.7610 (3)	−0.04786 (17)	0.0485 (7)
H4A	1.0529	0.6727	−0.0237	0.058*
N2	0.5383 (4)	1.5173 (3)	−0.18266 (17)	0.0586 (7)
N3	0.4501 (4)	1.6420 (3)	−0.22037 (18)	0.0634 (8)
C8	0.9513 (4)	1.2398 (3)	−0.21355 (17)	0.0448 (7)
H8A	0.8438	1.2177	−0.2410	0.054*
C1	0.7540 (4)	1.0183 (3)	−0.12364 (18)	0.0479 (7)
H1A	0.6786	1.1034	−0.1503	0.057*
C5	1.0687 (4)	0.8622 (3)	−0.08842 (17)	0.0482 (7)
H5A	1.2064	0.8425	−0.0905	0.058*
C11	1.3249 (4)	1.2494 (3)	−0.37556 (16)	0.0417 (7)
C18	0.5918 (4)	1.7106 (3)	−0.25259 (18)	0.0484 (7)
C14	1.6529 (5)	1.3212 (4)	−0.45817 (19)	0.0539 (8)
C9	0.8691 (4)	1.3685 (3)	−0.15506 (17)	0.0485 (7)
H9A	0.7980	1.3305	−0.1107	0.058*
H9B	0.9790	1.3984	−0.1346	0.058*
C22	0.9514 (4)	1.6647 (3)	−0.25652 (19)	0.0510 (8)
H22A	1.0754	1.6052	−0.2432	0.061*
C15	1.5886 (5)	1.3755 (4)	−0.3833 (2)	0.0581 (8)
H15A	1.6554	1.4369	−0.3599	0.070*
C21	0.9294 (6)	1.7981 (4)	−0.2997 (2)	0.0640 (9)
H21A	1.0418	1.8309	−0.3157	0.077*
C13	1.5503 (5)	1.2311 (4)	−0.49113 (19)	0.0620 (9)
H13A	1.5903	1.1943	−0.5419	0.074*
C16	1.4265 (5)	1.3409 (4)	−0.34183 (19)	0.0538 (8)
H16A	1.3859	1.3791	−0.2914	0.065*
C12	1.3898 (5)	1.1939 (4)	−0.45095 (19)	0.0556 (8)
H12A	1.3247	1.1314	−0.4744	0.067*
C19	0.5745 (6)	1.8472 (4)	−0.2986 (2)	0.0635 (9)
H19A	0.4518	1.9070	−0.3131	0.076*
C20	0.7445 (6)	1.8872 (4)	−0.3207 (2)	0.0700 (10)
H20A	0.7376	1.9768	−0.3507	0.084*
C23	1.8288 (5)	1.3588 (4)	−0.5021 (2)	0.0748 (11)
H23A	1.8520	1.3110	−0.5529	0.112*
H23B	1.9438	1.3214	−0.4721	0.112*
H23C	1.8032	1.4680	−0.5096	0.112*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0657 (3)	0.0510 (2)	0.0827 (3)	−0.01976 (17)	0.00767 (18)	0.01260 (17)
O2	0.0511 (12)	0.0408 (10)	0.0493 (12)	−0.0145 (9)	0.0068 (10)	0.0008 (9)
N1	0.0372 (14)	0.0429 (13)	0.0534 (15)	−0.0059 (11)	0.0009 (11)	−0.0022 (11)
O3	0.0652 (15)	0.0523 (13)	0.0687 (15)	−0.0269 (12)	0.0071 (12)	−0.0078 (11)
O1	0.0403 (14)	0.0751 (16)	0.0899 (18)	−0.0122 (11)	−0.0056 (12)	0.0310 (13)
C2	0.0351 (16)	0.0505 (17)	0.0577 (19)	−0.0072 (14)	−0.0024 (14)	0.0071 (15)
C3	0.0519 (19)	0.0412 (16)	0.0441 (17)	−0.0149 (14)	−0.0020 (14)	0.0012 (13)
C7	0.0394 (18)	0.0489 (17)	0.0500 (18)	−0.0084 (14)	0.0004 (14)	0.0043 (14)
C6	0.0401 (17)	0.0398 (15)	0.0419 (16)	−0.0064 (13)	−0.0020 (13)	0.0027 (13)
C17	0.0414 (17)	0.0361 (14)	0.0448 (17)	−0.0059 (13)	−0.0055 (13)	−0.0047 (12)
C10	0.0472 (18)	0.0363 (15)	0.0476 (17)	−0.0076 (14)	−0.0043 (14)	0.0067 (13)
C4	0.0449 (18)	0.0449 (17)	0.0495 (18)	−0.0018 (14)	−0.0060 (14)	0.0103 (14)
N2	0.0386 (15)	0.0616 (17)	0.0748 (19)	−0.0141 (13)	0.0098 (13)	−0.0108 (15)
N3	0.0378 (15)	0.0599 (18)	0.088 (2)	−0.0039 (14)	−0.0047 (15)	−0.0086 (16)
C8	0.0415 (17)	0.0447 (16)	0.0475 (17)	−0.0123 (13)	0.0012 (13)	0.0077 (13)
C1	0.0406 (17)	0.0445 (16)	0.0519 (18)	−0.0009 (13)	−0.0042 (14)	0.0089 (14)
C5	0.0363 (17)	0.0526 (18)	0.0518 (18)	−0.0051 (14)	−0.0052 (14)	0.0059 (14)
C11	0.0437 (17)	0.0367 (14)	0.0414 (16)	−0.0061 (13)	0.0005 (13)	0.0037 (12)
C18	0.0424 (18)	0.0449 (17)	0.0557 (19)	−0.0047 (14)	−0.0084 (14)	−0.0105 (14)
C14	0.0472 (19)	0.0560 (19)	0.055 (2)	−0.0107 (15)	0.0015 (15)	0.0099 (16)
C9	0.0479 (18)	0.0498 (17)	0.0435 (17)	−0.0075 (14)	0.0012 (14)	0.0056 (14)
C22	0.0407 (18)	0.0485 (17)	0.064 (2)	−0.0119 (14)	−0.0001 (15)	−0.0044 (15)
C15	0.056 (2)	0.060 (2)	0.064 (2)	−0.0253 (17)	−0.0023 (17)	−0.0009 (17)
C21	0.068 (2)	0.053 (2)	0.074 (2)	−0.0241 (18)	0.0064 (19)	−0.0016 (17)
C13	0.070 (2)	0.070 (2)	0.0427 (19)	−0.0167 (19)	0.0139 (16)	−0.0045 (16)
C16	0.055 (2)	0.0575 (19)	0.0499 (19)	−0.0171 (16)	0.0015 (15)	−0.0021 (15)
C12	0.066 (2)	0.0507 (18)	0.052 (2)	−0.0197 (16)	0.0011 (16)	−0.0063 (15)
C19	0.070 (2)	0.0463 (19)	0.067 (2)	0.0044 (17)	−0.0256 (19)	−0.0064 (16)
C20	0.098 (3)	0.0427 (18)	0.067 (2)	−0.013 (2)	−0.010 (2)	0.0054 (17)
C23	0.055 (2)	0.092 (3)	0.074 (3)	−0.020 (2)	0.0084 (19)	0.022 (2)

Geometric parameters (Å, º)

Br1—C3	1.898 (3)	C5—H5A	0.9300
O2—C10	1.355 (3)	C11—C16	1.387 (4)
O2—C8	1.431 (3)	C11—C12	1.389 (4)
N1—N2	1.360 (3)	C18—C19	1.415 (5)
N1—C17	1.371 (3)	C14—C13	1.377 (5)
N1—C9	1.441 (4)	C14—C15	1.378 (4)
O3—C10	1.203 (3)	C14—C23	1.498 (4)
O1—C7	1.209 (3)	C9—H9A	0.9700
C2—C3	1.374 (4)	C9—H9B	0.9700
C2—C1	1.385 (4)	C22—C21	1.362 (4)
C2—H2A	0.9300	C22—H22A	0.9300
C3—C4	1.381 (4)	C15—C16	1.388 (4)

C7—C6	1.488 (4)	C15—H15A	0.9300
C7—C8	1.533 (4)	C21—C20	1.393 (5)
C6—C1	1.383 (4)	C21—H21A	0.9300
C6—C5	1.390 (4)	C13—C12	1.379 (4)
C17—C18	1.387 (4)	C13—H13A	0.9300
C17—C22	1.391 (4)	C16—H16A	0.9300
C10—C11	1.469 (4)	C12—H12A	0.9300
C4—C5	1.379 (4)	C19—C20	1.353 (5)
C4—H4A	0.9300	C19—H19A	0.9300
N2—N3	1.299 (4)	C20—H20A	0.9300
N3—C18	1.371 (4)	C23—H23A	0.9600
C8—C9	1.523 (4)	C23—H23B	0.9600
C8—H8A	0.9800	C23—H23C	0.9600
C1—H1A	0.9300		

C10—O2—C8	116.1 (2)	N3—C18—C17	109.1 (3)
N2—N1—C17	110.0 (2)	N3—C18—C19	131.0 (3)
N2—N1—C9	119.3 (2)	C17—C18—C19	119.9 (3)
C17—N1—C9	130.7 (2)	C13—C14—C15	117.7 (3)
C3—C2—C1	119.0 (3)	C13—C14—C23	121.2 (3)
C3—C2—H2A	120.5	C15—C14—C23	121.1 (3)
C1—C2—H2A	120.5	N1—C9—C8	113.1 (2)
C2—C3—C4	121.3 (3)	N1—C9—H9A	109.0
C2—C3—Br1	119.9 (2)	C8—C9—H9A	109.0
C4—C3—Br1	118.8 (2)	N1—C9—H9B	109.0
O1—C7—C6	121.5 (3)	C8—C9—H9B	109.0
O1—C7—C8	118.6 (3)	H9A—C9—H9B	107.8
C6—C7—C8	119.9 (2)	C21—C22—C17	116.2 (3)
C1—C6—C5	118.5 (3)	C21—C22—H22A	121.9
C1—C6—C7	123.4 (3)	C17—C22—H22A	121.9
C5—C6—C7	118.1 (3)	C14—C15—C16	121.6 (3)
N1—C17—C18	103.8 (2)	C14—C15—H15A	119.2
N1—C17—C22	133.8 (3)	C16—C15—H15A	119.2
C18—C17—C22	122.5 (3)	C22—C21—C20	122.4 (3)
O3—C10—O2	122.3 (3)	C22—C21—H21A	118.8
O3—C10—C11	125.2 (3)	C20—C21—H21A	118.8
O2—C10—C11	112.5 (2)	C14—C13—C12	121.8 (3)
C5—C4—C3	119.0 (3)	C14—C13—H13A	119.1
C5—C4—H4A	120.5	C12—C13—H13A	119.1
C3—C4—H4A	120.5	C11—C16—C15	120.1 (3)
N3—N2—N1	108.7 (2)	C11—C16—H16A	119.9
N2—N3—C18	108.5 (2)	C15—C16—H16A	119.9
O2—C8—C9	105.7 (2)	C13—C12—C11	120.2 (3)
O2—C8—C7	109.4 (2)	C13—C12—H12A	119.9
C9—C8—C7	109.5 (2)	C11—C12—H12A	119.9
O2—C8—H8A	110.7	C20—C19—C18	117.1 (3)
C9—C8—H8A	110.7	C20—C19—H19A	121.4
C7—C8—H8A	110.7	C18—C19—H19A	121.4

C6—C1—C2	121.2 (3)	C19—C20—C21	122.0 (3)
C6—C1—H1A	119.4	C19—C20—H20A	119.0
C2—C1—H1A	119.4	C21—C20—H20A	119.0
C4—C5—C6	121.1 (3)	C14—C23—H23A	109.5
C4—C5—H5A	119.5	C14—C23—H23B	109.5
C6—C5—H5A	119.5	H23A—C23—H23B	109.5
C16—C11—C12	118.5 (3)	C14—C23—H23C	109.5
C16—C11—C10	121.5 (3)	H23A—C23—H23C	109.5
C12—C11—C10	119.9 (3)	H23B—C23—H23C	109.5

C1—C2—C3—C4	−1.9 (5)	O2—C10—C11—C16	17.0 (4)
C1—C2—C3—Br1	178.4 (2)	O3—C10—C11—C12	14.9 (5)
O1—C7—C6—C1	178.7 (3)	O2—C10—C11—C12	−166.0 (3)
C8—C7—C6—C1	0.5 (4)	N2—N3—C18—C17	0.0 (4)
O1—C7—C6—C5	−3.3 (5)	N2—N3—C18—C19	−179.9 (3)
C8—C7—C6—C5	178.6 (3)	N1—C17—C18—N3	0.3 (3)
N2—N1—C17—C18	−0.5 (3)	C22—C17—C18—N3	−178.6 (3)
C9—N1—C17—C18	177.8 (3)	N1—C17—C18—C19	−179.7 (3)
N2—N1—C17—C22	178.2 (3)	C22—C17—C18—C19	1.4 (4)
C9—N1—C17—C22	−3.5 (5)	N2—N1—C9—C8	94.9 (3)
C8—O2—C10—O3	11.8 (4)	C17—N1—C9—C8	−83.2 (4)
C8—O2—C10—C11	−167.4 (2)	O2—C8—C9—N1	69.6 (3)
C2—C3—C4—C5	3.0 (5)	C7—C8—C9—N1	−172.6 (2)
Br1—C3—C4—C5	−177.4 (2)	N1—C17—C22—C21	−178.8 (3)
C17—N1—N2—N3	0.6 (3)	C18—C17—C22—C21	−0.3 (4)
C9—N1—N2—N3	−178.0 (3)	C13—C14—C15—C16	0.2 (5)
N1—N2—N3—C18	−0.4 (3)	C23—C14—C15—C16	−179.7 (3)
C10—O2—C8—C9	−172.5 (2)	C17—C22—C21—C20	−0.7 (5)
C10—O2—C8—C7	69.6 (3)	C15—C14—C13—C12	−0.8 (5)
O1—C7—C8—O2	18.9 (4)	C23—C14—C13—C12	179.1 (3)
C6—C7—C8—O2	−163.0 (2)	C12—C11—C16—C15	0.2 (5)
O1—C7—C8—C9	−96.6 (3)	C10—C11—C16—C15	177.3 (3)
C6—C7—C8—C9	81.6 (3)	C14—C15—C16—C11	0.1 (5)
C5—C6—C1—C2	2.4 (5)	C14—C13—C12—C11	1.1 (5)
C7—C6—C1—C2	−179.6 (3)	C16—C11—C12—C13	−0.7 (5)
C3—C2—C1—C6	−0.8 (5)	C10—C11—C12—C13	−177.9 (3)
C3—C4—C5—C6	−1.3 (5)	N3—C18—C19—C20	178.6 (3)
C1—C6—C5—C4	−1.3 (4)	C17—C18—C19—C20	−1.4 (5)
C7—C6—C5—C4	−179.4 (3)	C18—C19—C20—C21	0.4 (5)
O3—C10—C11—C16	−162.2 (3)	C22—C21—C20—C19	0.7 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15*A*···*Cg*1^{i}	0.93	2.86	3.596 (1)	138
C2—H2*A*···O1^{ii}	0.93	2.56	3.292 (4)	137

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