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## 2-(1*H*-Benzotriazol-1-yl)-1-(4-ethylbenzoyl)ethyl 2-chlorobenzoate

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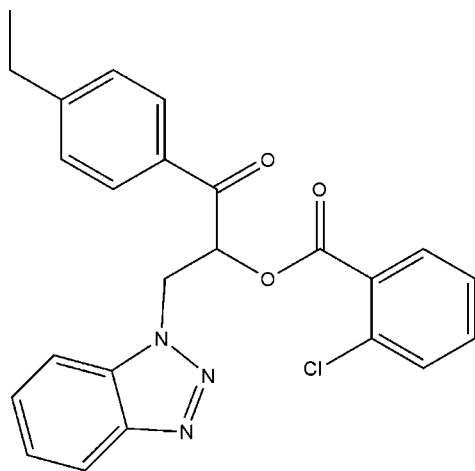
Received 9 July 2009; accepted 12 August 2009

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.006$  Å;  $R$  factor = 0.057;  $wR$  factor = 0.158; data-to-parameter ratio = 18.5.

In the crystal structure of the title compound,  $\text{C}_{24}\text{H}_{20}\text{ClN}_3\text{O}_3$ , weak intermolecular  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds link the molecules into chains extended along the  $a$  axis. The crystal studied was found to be an inversion twin.

### Related literature

For background to the pharmacological activity of 1*H*-benzotriazole and its derivative, see Chen & Wu (2005). For reference structural data, see: Allen *et al.* (1987).



### Experimental

#### Crystal data

$\text{C}_{24}\text{H}_{20}\text{ClN}_3\text{O}_3$   
 $M_r = 433.88$   
 Orthorhombic,  $P2_12_12_1$   
 $a = 9.433$  (2) Å  
 $b = 14.824$  (4) Å  
 $c = 15.239$  (4) Å  
 $V = 2131.0$  (10) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.21$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.15 \times 0.12 \times 0.10$  mm

#### Data collection

Bruker SMART CCD diffractometer  
 Absorption correction: none  
 13991 measured reflections  
 5212 independent reflections  
 2174 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.078$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.057$   
 $wR(F^2) = 0.158$   
 $S = 0.91$   
 5212 reflections  
 281 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.22$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.20$  e Å<sup>-3</sup>  
 Absolute structure: Flack (1983),  
 2244 Friedel pairs  
 Flack parameter: 0.57 (12)

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C7}-\text{H7B}\cdots\text{O3}^{\text{i}}$	0.97	2.51	3.162 (4)	125
$\text{C8}-\text{H8A}\cdots\text{O2}^{\text{ii}}$	0.98	2.42	3.397 (5)	171
$\text{C11}-\text{H11A}\cdots\text{O2}^{\text{ii}}$	0.93	2.56	3.431 (5)	155

Symmetry codes: (i)  $x - \frac{1}{2}, -y + \frac{3}{2}, -z$ ; (ii)  $x + \frac{1}{2}, -y + \frac{3}{2}, -z$ .

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5022).

### References

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## supporting information

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**2-(1*H*-Benzotriazol-1-yl)-1-(4-ethylbenzoyl)ethyl 2-chlorobenzoate****Wu-Lan Zeng and Fang-Fang Jian****S1. Comment**

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

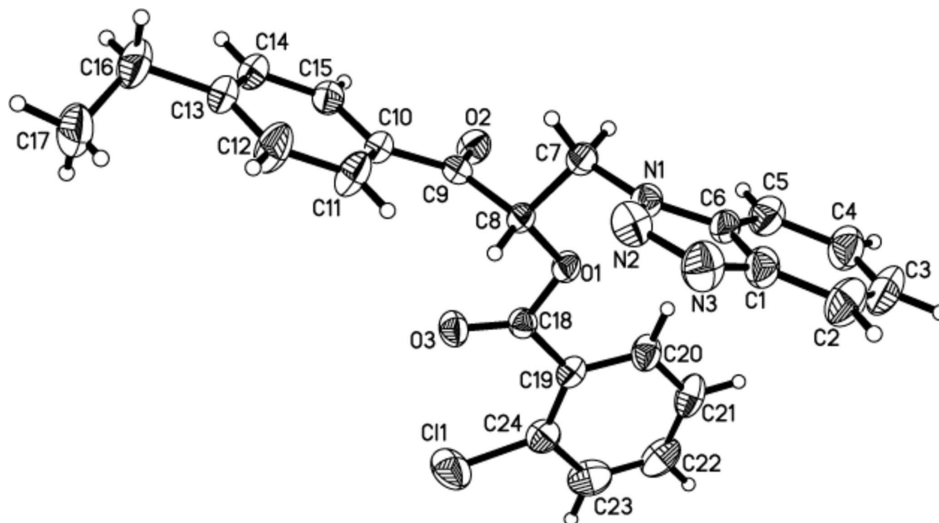
All the bond lengths and angles in (I) are within their normal ranges (Allen *et al.*, 1987). The benzotriazole ring system is essentially planar, with a dihedral angle of 1.97 (1)° between the triazole ring (atoms N1—N3/C1/C6) and the C1—C6 benzene ring. The dihedral angles between the mean planes of the benzotriazole system and the C10—C15 and C19—C24 aromatic rings are 9.25 (1)° and 87.55 (1)°, respectively. The dihedral angle between rings C10—C15 and C19—C24 is 85.25 (2)°. Molecule (I) is chiral: atom C8 has *S* configuration, but refinement showed the crystal to be a racemic twin.

**S2. 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-(4-ethylphenyl)propan-1-one (5.58 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 saturated sodium bicarbonate solution and brine, dried over anhydrous magnesium sulfate and the chloroform solution filtered. It was cooled with ice-water, and then an acetone solution (10 ml) of 2-chlorobenzoic acid (3.1 g, 0.02 mol) and triethylamine (2.8 ml) was added. The mixture was stirred with ice-water for 6 h. The solution was then filtered and concentrated. Colourless blocks of (I) were obtained by slow evaporation of an petroleum aether-ethylacetate (3:1 *v/v*) solution at room temperature over a period of one week.

**S3. Refinement**

The H atoms were geometrically placed (C—H = 0.93–0.97 Å), and refined as riding with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  or  $1.5U_{\text{eq}}(\text{methyl C})$ .

**Figure 1**

The molecular structure of (I), drawn with 30% probability ellipsoids (arbitrary spheres for the H atoms).

### 2-(1*H*-Benzotriazol-1-yl)-1-(4-ethylbenzoyl)ethyl 2-chlorobenzoate

#### Crystal data

$C_{24}H_{20}ClN_3O_3$

$M_r = 433.88$

Orthorhombic,  $P2_12_12_1$

Hall symbol: P 2ac 2ab

$a = 9.433$  (2) Å

$b = 14.824$  (4) Å

$c = 15.239$  (4) Å

$V = 2131.0$  (10) Å<sup>3</sup>

$Z = 4$

$F(000) = 904$

$D_x = 1.352$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 5212 reflections

$\theta = 1.9$ – $28.3^\circ$

$\mu = 0.21$  mm<sup>-1</sup>

$T = 293$  K

Block, colourless

$0.15 \times 0.12 \times 0.10$  mm

#### Data collection

Bruker SMART CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\omega$  scans

13991 measured reflections

5212 independent reflections

2174 reflections with  $I > 2\sigma(I)$

$R_{int} = 0.078$

$\theta_{max} = 28.3^\circ$ ,  $\theta_{min} = 1.9^\circ$

$h = -12 \rightarrow 12$

$k = -19 \rightarrow 17$

$l = -20 \rightarrow 13$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.057$

$wR(F^2) = 0.158$

$S = 0.91$

5212 reflections

281 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

$w = 1/[\sigma^2(F_o^2) + (0.0626P)^2]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.22$  e Å<sup>-3</sup>

$\Delta\rho_{min} = -0.20$  e Å<sup>-3</sup>

Extinction correction: *SHELXL97* (Sheldrick,  
2008),  $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0034 (10)

Absolute structure: Flack (1983), 2214 Friedel pairs

Absolute structure parameter: 0.57 (12)

### 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 ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	0.15025 (14)	0.62148 (8)	0.24883 (9)	0.0933 (5)
O1	-0.1687 (2)	0.61438 (14)	0.03013 (16)	0.0470 (6)
O2	-0.3655 (3)	0.73734 (15)	0.08575 (17)	0.0573 (7)
O3	-0.0410 (3)	0.69848 (17)	0.12131 (18)	0.0572 (7)
N1	-0.2042 (3)	0.6104 (2)	-0.15765 (19)	0.0497 (8)
N2	-0.1122 (4)	0.6446 (2)	-0.2173 (2)	0.0660 (10)
N3	-0.0555 (4)	0.5770 (3)	-0.2603 (2)	0.0788 (11)
C1	-0.1124 (5)	0.4984 (3)	-0.2287 (3)	0.0627 (12)
C2	-0.0891 (5)	0.4096 (3)	-0.2526 (3)	0.0803 (14)
H2B	-0.0234	0.3952	-0.2958	0.096*
C3	-0.1639 (7)	0.3446 (3)	-0.2116 (3)	0.0887 (17)
H3B	-0.1497	0.2846	-0.2270	0.106*
C4	-0.2615 (6)	0.3655 (3)	-0.1468 (3)	0.0806 (14)
H4A	-0.3124	0.3190	-0.1206	0.097*
C5	-0.2858 (5)	0.4534 (3)	-0.1199 (3)	0.0669 (12)
H5A	-0.3507	0.4675	-0.0760	0.080*
C6	-0.2070 (4)	0.5187 (3)	-0.1626 (3)	0.0502 (10)
C7	-0.2789 (4)	0.6705 (2)	-0.0990 (2)	0.0508 (10)
H7A	-0.3658	0.6415	-0.0799	0.061*
H7B	-0.3047	0.7248	-0.1308	0.061*
C8	-0.1931 (4)	0.6963 (2)	-0.0194 (2)	0.0430 (9)
H8A	-0.1022	0.7221	-0.0379	0.052*
C9	-0.2747 (4)	0.7649 (2)	0.0346 (3)	0.0433 (9)
C10	-0.2528 (4)	0.8626 (2)	0.0197 (2)	0.0433 (9)
C11	-0.1516 (5)	0.8960 (3)	-0.0356 (3)	0.0705 (13)
H11A	-0.0911	0.8566	-0.0649	0.085*
C12	-0.1383 (5)	0.9887 (3)	-0.0485 (3)	0.0804 (15)
H12A	-0.0683	1.0103	-0.0860	0.097*
C13	-0.2257 (5)	1.0486 (2)	-0.0072 (3)	0.0656 (12)
C14	-0.3253 (5)	1.0147 (3)	0.0490 (3)	0.0650 (13)
H14A	-0.3849	1.0542	0.0789	0.078*
C15	-0.3386 (4)	0.9232 (2)	0.0622 (3)	0.0545 (10)
H15A	-0.4073	0.9020	0.1009	0.065*

C16	-0.2116 (6)	1.1492 (3)	-0.0229 (4)	0.0990 (18)
H16A	-0.2517	1.1628	-0.0800	0.119*
H16B	-0.2687	1.1803	0.0205	0.119*
C17	-0.0676 (6)	1.1865 (3)	-0.0198 (4)	0.109 (2)
H17A	-0.0709	1.2501	-0.0311	0.164*
H17B	-0.0099	1.1575	-0.0634	0.164*
H17C	-0.0276	1.1761	0.0373	0.164*
C18	-0.0826 (4)	0.6257 (2)	0.1005 (2)	0.0443 (9)
C19	-0.0495 (4)	0.5386 (2)	0.1438 (2)	0.0459 (10)
C20	-0.1196 (5)	0.4611 (2)	0.1187 (3)	0.0602 (11)
H20A	-0.1879	0.4645	0.0748	0.072*
C21	-0.0906 (6)	0.3783 (3)	0.1573 (3)	0.0742 (14)
H21A	-0.1399	0.3270	0.1397	0.089*
C22	0.0106 (6)	0.3724 (3)	0.2212 (3)	0.0772 (14)
H22A	0.0306	0.3170	0.2471	0.093*
C23	0.0820 (5)	0.4473 (3)	0.2466 (3)	0.0840 (15)
H23A	0.1517	0.4428	0.2895	0.101*
C24	0.0519 (5)	0.5315 (3)	0.2090 (3)	0.0589 (11)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cl1	0.1010 (9)	0.0888 (9)	0.0902 (9)	-0.0149 (8)	-0.0451 (8)	0.0174 (8)
O1	0.0570 (15)	0.0334 (13)	0.0505 (15)	0.0011 (12)	-0.0078 (13)	0.0052 (12)
O2	0.0568 (17)	0.0499 (15)	0.0652 (19)	0.0002 (14)	0.0106 (16)	0.0067 (14)
O3	0.0709 (18)	0.0426 (15)	0.0583 (17)	-0.0093 (14)	-0.0145 (15)	0.0040 (14)
N1	0.057 (2)	0.0464 (19)	0.0452 (18)	0.0041 (16)	-0.0044 (17)	-0.0047 (16)
N2	0.074 (2)	0.073 (2)	0.051 (2)	-0.011 (2)	0.004 (2)	0.001 (2)
N3	0.091 (3)	0.086 (3)	0.060 (2)	-0.002 (2)	0.016 (2)	-0.015 (2)
C1	0.078 (3)	0.059 (3)	0.052 (3)	0.005 (3)	-0.005 (2)	-0.011 (2)
C2	0.103 (4)	0.078 (3)	0.060 (3)	0.020 (3)	0.019 (3)	-0.011 (3)
C3	0.131 (5)	0.060 (3)	0.075 (3)	0.034 (3)	0.003 (4)	-0.015 (3)
C4	0.108 (4)	0.051 (3)	0.083 (3)	0.006 (3)	-0.014 (3)	-0.001 (3)
C5	0.084 (3)	0.058 (3)	0.059 (3)	0.010 (2)	0.000 (3)	0.001 (2)
C6	0.058 (3)	0.046 (2)	0.046 (2)	0.009 (2)	-0.009 (2)	-0.008 (2)
C7	0.057 (2)	0.045 (2)	0.051 (2)	0.0063 (19)	-0.008 (2)	-0.0040 (19)
C8	0.049 (2)	0.0317 (18)	0.049 (2)	0.0025 (16)	-0.0073 (19)	0.0034 (18)
C9	0.039 (2)	0.046 (2)	0.044 (2)	-0.0013 (18)	-0.006 (2)	-0.0013 (19)
C10	0.049 (2)	0.036 (2)	0.045 (2)	0.0026 (18)	0.0024 (19)	0.0004 (18)
C11	0.088 (3)	0.040 (2)	0.084 (3)	0.009 (2)	0.022 (3)	0.007 (2)
C12	0.094 (4)	0.044 (3)	0.104 (4)	0.000 (3)	0.037 (3)	0.013 (3)
C13	0.069 (3)	0.037 (2)	0.091 (3)	0.003 (2)	-0.009 (3)	-0.002 (2)
C14	0.063 (3)	0.044 (3)	0.088 (3)	0.011 (2)	-0.004 (3)	-0.014 (2)
C15	0.053 (2)	0.050 (2)	0.061 (2)	0.000 (2)	0.001 (2)	-0.004 (2)
C16	0.107 (4)	0.039 (2)	0.151 (5)	-0.004 (3)	-0.003 (4)	0.013 (3)
C17	0.131 (5)	0.053 (3)	0.144 (5)	-0.018 (3)	-0.027 (4)	0.011 (3)
C18	0.044 (2)	0.042 (2)	0.046 (2)	-0.0026 (19)	0.0019 (19)	0.000 (2)
C19	0.057 (2)	0.042 (2)	0.039 (2)	0.007 (2)	0.0058 (19)	0.0021 (18)

C20	0.084 (3)	0.044 (2)	0.053 (2)	0.002 (2)	-0.009 (2)	0.001 (2)
C21	0.109 (4)	0.037 (2)	0.076 (3)	0.000 (3)	0.013 (3)	0.003 (2)
C22	0.101 (4)	0.056 (3)	0.074 (3)	0.021 (3)	0.017 (3)	0.027 (3)
C23	0.092 (4)	0.085 (3)	0.075 (3)	0.019 (3)	-0.014 (3)	0.029 (3)
C24	0.068 (3)	0.054 (2)	0.054 (3)	0.005 (2)	-0.002 (2)	0.012 (2)

*Geometric parameters (Å, °)*

C11—C24	1.734 (4)	C10—C15	1.373 (5)
O1—C18	1.355 (4)	C11—C12	1.394 (5)
O1—C8	1.448 (4)	C11—H11A	0.9300
O2—C9	1.228 (4)	C12—C13	1.364 (6)
O3—C18	1.191 (4)	C12—H12A	0.9300
N1—N2	1.355 (4)	C13—C14	1.368 (6)
N1—C6	1.361 (4)	C13—C16	1.516 (5)
N1—C7	1.445 (4)	C14—C15	1.378 (5)
N2—N3	1.312 (4)	C14—H14A	0.9300
N3—C1	1.371 (5)	C15—H15A	0.9300
C1—C6	1.380 (6)	C16—C17	1.468 (7)
C1—C2	1.382 (5)	C16—H16A	0.9700
C2—C3	1.348 (6)	C16—H16B	0.9700
C2—H2B	0.9300	C17—H17A	0.9600
C3—C4	1.385 (7)	C17—H17B	0.9600
C3—H3B	0.9300	C17—H17C	0.9600
C4—C5	1.385 (6)	C18—C19	1.483 (5)
C4—H4A	0.9300	C19—C20	1.379 (5)
C5—C6	1.383 (5)	C19—C24	1.383 (6)
C5—H5A	0.9300	C20—C21	1.389 (5)
C7—C8	1.508 (5)	C20—H20A	0.9300
C7—H7A	0.9700	C21—C22	1.367 (7)
C7—H7B	0.9700	C21—H21A	0.9300
C8—C9	1.518 (5)	C22—C23	1.355 (6)
C8—H8A	0.9800	C22—H22A	0.9300
C9—C10	1.480 (5)	C23—C24	1.403 (6)
C10—C11	1.367 (5)	C23—H23A	0.9300
C18—O1—C8	113.8 (2)	C13—C12—C11	121.5 (4)
N2—N1—C6	110.5 (3)	C13—C12—H12A	119.2
N2—N1—C7	119.8 (3)	C11—C12—H12A	119.2
C6—N1—C7	129.8 (3)	C12—C13—C14	117.7 (4)
N3—N2—N1	108.1 (3)	C12—C13—C16	121.0 (5)
N2—N3—C1	108.3 (3)	C14—C13—C16	121.3 (4)
N3—C1—C6	108.9 (4)	C13—C14—C15	121.1 (4)
N3—C1—C2	130.9 (4)	C13—C14—H14A	119.5
C6—C1—C2	120.2 (4)	C15—C14—H14A	119.5
C3—C2—C1	118.4 (4)	C10—C15—C14	121.5 (4)
C3—C2—H2B	120.8	C10—C15—H15A	119.3
C1—C2—H2B	120.8	C14—C15—H15A	119.3

C2—C3—C4	121.2 (4)	C17—C16—C13	116.5 (4)
C2—C3—H3B	119.4	C17—C16—H16A	108.2
C4—C3—H3B	119.4	C13—C16—H16A	108.2
C5—C4—C3	122.1 (5)	C17—C16—H16B	108.2
C5—C4—H4A	118.9	C13—C16—H16B	108.2
C3—C4—H4A	118.9	H16A—C16—H16B	107.3
C6—C5—C4	115.5 (4)	C16—C17—H17A	109.5
C6—C5—H5A	122.3	C16—C17—H17B	109.5
C4—C5—H5A	122.3	H17A—C17—H17B	109.5
N1—C6—C1	104.2 (4)	C16—C17—H17C	109.5
N1—C6—C5	133.1 (4)	H17A—C17—H17C	109.5
C1—C6—C5	122.6 (4)	H17B—C17—H17C	109.5
N1—C7—C8	113.0 (3)	O3—C18—O1	121.4 (3)
N1—C7—H7A	109.0	O3—C18—C19	126.9 (4)
C8—C7—H7A	109.0	O1—C18—C19	111.7 (3)
N1—C7—H7B	109.0	C20—C19—C24	117.9 (3)
C8—C7—H7B	109.0	C20—C19—C18	120.0 (4)
H7A—C7—H7B	107.8	C24—C19—C18	122.1 (3)
O1—C8—C7	107.0 (3)	C19—C20—C21	121.6 (4)
O1—C8—C9	111.0 (3)	C19—C20—H20A	119.2
C7—C8—C9	109.5 (3)	C21—C20—H20A	119.2
O1—C8—H8A	109.8	C22—C21—C20	119.7 (4)
C7—C8—H8A	109.8	C22—C21—H21A	120.1
C9—C8—H8A	109.8	C20—C21—H21A	120.1
O2—C9—C10	121.3 (3)	C23—C22—C21	119.9 (4)
O2—C9—C8	118.4 (3)	C23—C22—H22A	120.0
C10—C9—C8	120.1 (3)	C21—C22—H22A	120.0
C11—C10—C15	117.8 (3)	C22—C23—C24	120.8 (4)
C11—C10—C9	123.1 (3)	C22—C23—H23A	119.6
C15—C10—C9	119.1 (3)	C24—C23—H23A	119.6
C10—C11—C12	120.4 (4)	C19—C24—C23	120.1 (4)
C10—C11—H11A	119.8	C19—C24—C11	124.3 (3)
C12—C11—H11A	119.8	C23—C24—C11	115.7 (4)

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C7—H7B $\cdots$ O3 <sup>i</sup>	0.97	2.51	3.162 (4)	125
C8—H8A $\cdots$ O2 <sup>ii</sup>	0.98	2.42	3.397 (5)	171
C11—H11A $\cdots$ O2 <sup>ii</sup>	0.93	2.56	3.431 (5)	155

Symmetry codes: (i)  $x-1/2, -y+3/2, -z$ ; (ii)  $x+1/2, -y+3/2, -z$ .