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8-Bromo-3-(4-ethylphenyl)-1-phenyl-3,3a,4,9b-tetrahydro-1*H*-chromeno[4,3-*c*]isoxazole-3a-carbonitrile

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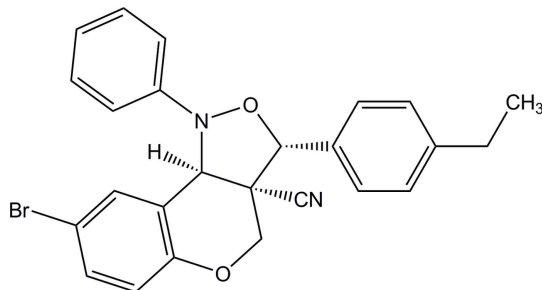
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Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.044; wR factor = 0.123; data-to-parameter ratio = 25.2.

In the title compound, $\text{C}_{25}\text{H}_{21}\text{BrN}_2\text{O}_2$, the fused isoxazolidine ring adopts an envelope conformation with the N atom at the flap and the mean plane of the ring makes dihedral angles of 54.37 (12) and 87.32 (13)°, respectively, with the adjacent phenyl and benzene rings. The tetrahydropyran ring has a half-chair conformation. In the crystal, molecules are linked into a double-column structure along the b -axis direction through weak $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\pi$ interactions.

Related literature

For the biological activity of cyanoacrylates, see: Zhang *et al.* (2009); Obniska *et al.* (2005). For related structures, see: Ye *et al.* (2009); Suresh *et al.* (2012); Kanchanadevi *et al.* (2013).



Experimental

Crystal data

$\text{C}_{25}\text{H}_{21}\text{BrN}_2\text{O}_2$
 $M_r = 461.35$
 Triclinic, $P\bar{1}$
 $a = 9.8813$ (3) Å
 $b = 9.9921$ (3) Å
 $c = 11.1587$ (3) Å
 $\alpha = 94.125$ (2)°
 $\beta = 92.196$ (2)°
 $\gamma = 101.500$ (2)°
 $V = 1075.27$ (5) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 1.94$ mm⁻¹
 $T = 295$ K
 $0.25 \times 0.20 \times 0.15$ mm

Data collection

Bruker APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.620$, $T_{\max} = 0.748$
 27480 measured reflections
 6895 independent reflections
 4405 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.031$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.123$
 $S = 1.02$
 6895 reflections
 274 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.54$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.81$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

Cg3, Cg4 and Cg5 are the centroids of the C1–C4/C8/C9, C10–C15 and C17–C22 rings, respectively.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
C11–H11 \cdots O1 ⁱ	0.93	2.57	3.475 (2)	165
C3–H3 \cdots Cg5 ⁱⁱ	0.93	2.78	3.491 (3)	134
C5–H5B \cdots Cg3 ⁱ	0.97	2.86	3.730 (4)	149
C22–H22 \cdots Cg4 ⁱⁱⁱ	0.93	2.95	3.628 (3)	131

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

Data collection: APEX2 (Bruker, 2008); cell refinement: SAINT (Bruker, 2008); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: PLATON (Spek, 2009); software used to prepare material for publication: SHELXL97.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS5299).

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supplementary materials

Acta Cryst. (2013). E69, o1533 [doi:10.1107/S1600536813023982]

8-Bromo-3-(4-ethylphenyl)-1-phenyl-3,3a,4,9b-tetrahydro-1H-chromeno[4,3-c]isoxazole-3a-carbonitrile

J. Kanchanadevi, G. Anbalagan, J. Srinivasan, M. Bakthadoss, B. Gunasekaran and V. Manivannan

1. Comment

Cyanoacrylates and its derivatives have been widely used as agrochemicals (Zhang *et al.*, 2009) and an important intermediate in drugs synthesis (Obniska *et al.*, 2005).

The geometric parameters of the title molecule (Fig. 1) agree well with reported similar structures (Ye *et al.*, 2009; Suresh *et al.*, 2012; Kanchanadevi *et al.*, 2013). The crystal packing is controlled by weak intermolecular C—H \cdots O and C—H \cdots π (C3—H3 \cdots Cg5ⁱⁱ, C5—H5B \cdots Cg3ⁱ and C22—H22 \cdots Cg4ⁱⁱⁱ; symmetry codes as in Table 1; Cg3, Cg4 and Cg5 are the centroids of the rings defined by the atoms C1—C4/C8/C9, C10—C15 and C17—C22, respectively) interactions.

2. Experimental

A mixture of (*E*)-2-[(4-bromo-2-formylphenoxy)methyl]-3-(4-ethylphenyl)acrylonitrile (2 mmol, 0.75 g) and *N*-phenylhydroxylamine (3 mmol, 0.33 g) in ethanol (10 ml) was refluxed for 6 h. After the completion of the reaction as indicated by TLC, the reaction mixture was concentrated and the resulting crude mass was diluted with water (15 ml) and extracted with ethyl acetate (3 \times 15 ml). The combined organic layer was washed with brine (3 \times 15 ml) and dried over anhydrous Na₂SO₄, solvent was removed under reduced pressure. The crude mass was purified by column chromatography on silica gel (Acme 100–200 mesh), using ethyl acetate–hexane (1:9) to afford the pure compound as a colourless solid in 82% yield and melting point 171–173 °C.

3. Refinement

H atoms were positioned geometrically (C—H = 0.93–0.98 Å) and refined using riding model with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{C}_{\text{methyl}})$.

Computing details

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINTE* (Bruker, 2008); data reduction: *SAINTE* (Bruker, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

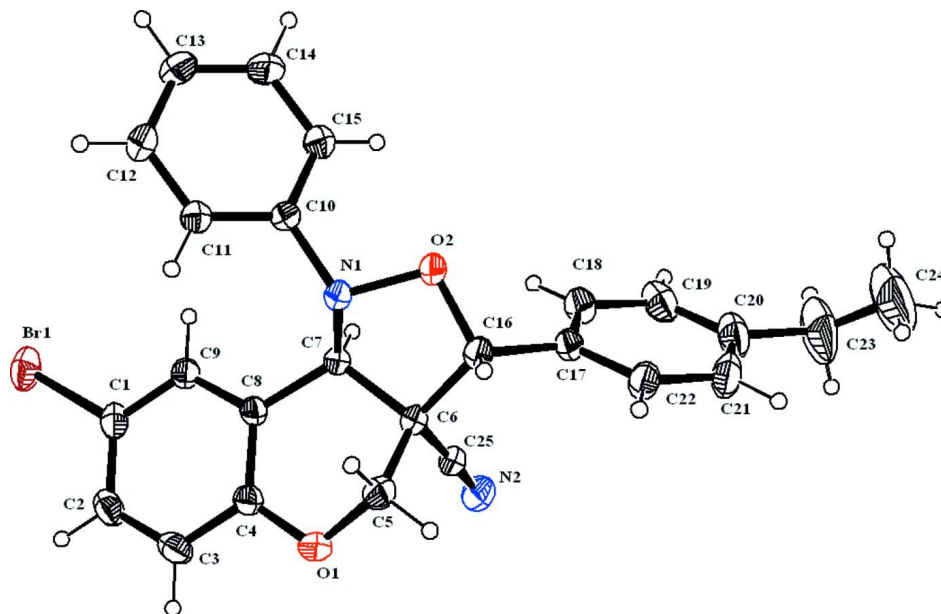


Figure 1

The molecular structure of the title compound, with atom labels and 30% probability displacement ellipsoids for non-H atoms.

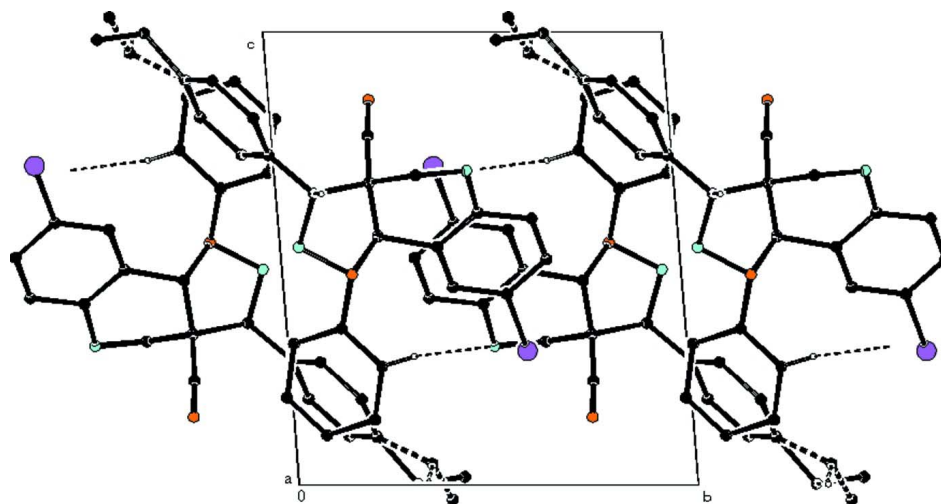


Figure 2

A packing diagram of the title compound, viewed down the *a* axis. Hydrogen bonds are shown as dashed lines.

8-Bromo-3-(4-ethylphenyl)-1-phenyl-3,3a,4,9b-tetrahydro-1H-chromeno[4,3-c]isoxazole-3a-carbonitrile

Crystal data

$C_{25}H_{21}BrN_2O_2$

$M_r = 461.35$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 9.8813(3)\ \text{\AA}$

$b = 9.9921(3)\ \text{\AA}$

$c = 11.1587(3)\ \text{\AA}$

$\alpha = 94.125(2)^\circ$

$\beta = 92.196(2)^\circ$

$\gamma = 101.500(2)^\circ$

$V = 1075.27(5)\ \text{\AA}^3$

$Z = 2$

$F(000) = 472$

$D_x = 1.425\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
 Cell parameters from 4405 reflections
 $\theta = 2.1\text{--}31.1^\circ$
 $\mu = 1.94 \text{ mm}^{-1}$

$T = 295 \text{ K}$
 Block, colourless
 $0.25 \times 0.20 \times 0.15 \text{ mm}$

Data collection

Bruker APEXII CCD
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 Detector resolution: 0 pixels mm^{-1}
 ω and φ scans
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.620$, $T_{\max} = 0.748$

27480 measured reflections
 6895 independent reflections
 4405 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.031$
 $\theta_{\max} = 31.1^\circ$, $\theta_{\min} = 2.1^\circ$
 $h = -13 \rightarrow 14$
 $k = -14 \rightarrow 14$
 $l = -16 \rightarrow 15$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.123$
 $S = 1.02$
 6895 reflections
 274 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
 $w = 1/[\sigma^2(F_o^2) + (0.0578P)^2 + 0.3505P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.54 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.81 \text{ e \AA}^{-3}$

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.04591 (3)	0.59905 (3)	0.29647 (2)	0.06392 (11)
O1	0.42095 (16)	0.48260 (14)	0.69339 (13)	0.0480 (4)
O2	0.32836 (18)	0.04730 (14)	0.52461 (12)	0.0479 (4)
N1	0.33533 (18)	0.17431 (16)	0.46483 (14)	0.0387 (4)
C6	0.3363 (2)	0.23582 (19)	0.66704 (16)	0.0366 (4)
C8	0.2571 (2)	0.39431 (18)	0.52539 (16)	0.0350 (4)
N2	0.1838 (2)	0.2514 (2)	0.85005 (17)	0.0566 (5)
C7	0.2565 (2)	0.24777 (18)	0.54874 (15)	0.0337 (4)
H7	0.1611	0.1965	0.5498	0.040*
C16	0.3846 (2)	0.0964 (2)	0.64292 (17)	0.0417 (4)
H16	0.4857	0.1146	0.6425	0.050*
C10	0.2740 (2)	0.13817 (19)	0.34525 (16)	0.0366 (4)
C12	0.2584 (2)	0.2032 (2)	0.14426 (18)	0.0490 (5)
H12	0.2816	0.2674	0.0883	0.059*
C17	0.3385 (2)	-0.0105 (2)	0.72803 (18)	0.0422 (4)
C9	0.1687 (2)	0.4248 (2)	0.43612 (17)	0.0390 (4)
H9	0.1143	0.3544	0.3861	0.047*
C5	0.4613 (2)	0.3539 (2)	0.68345 (19)	0.0449 (5)
H5A	0.5157	0.3445	0.7554	0.054*
H5B	0.5188	0.3499	0.6153	0.054*
C22	0.4339 (3)	-0.0410 (2)	0.81004 (19)	0.0512 (5)
H22	0.5263	0.0027	0.8100	0.061*

C25	0.2495 (2)	0.2419 (2)	0.77047 (17)	0.0408 (4)
C4	0.3342 (2)	0.50191 (19)	0.60093 (17)	0.0391 (4)
C15	0.1848 (2)	0.0155 (2)	0.31184 (19)	0.0480 (5)
H15	0.1581	-0.0473	0.3684	0.058*
C13	0.1712 (3)	0.0798 (3)	0.1099 (2)	0.0544 (6)
H13	0.1368	0.0599	0.0305	0.065*
C11	0.3113 (2)	0.2318 (2)	0.26118 (17)	0.0419 (4)
H11	0.3723	0.3142	0.2836	0.050*
C14	0.1354 (3)	-0.0133 (2)	0.1927 (2)	0.0570 (6)
H14	0.0772	-0.0970	0.1691	0.068*
C3	0.3218 (2)	0.6360 (2)	0.5880 (2)	0.0484 (5)
H3	0.3717	0.7065	0.6406	0.058*
C21	0.3925 (3)	-0.1363 (3)	0.8921 (2)	0.0663 (7)
H21	0.4575	-0.1547	0.9477	0.080*
C2	0.2369 (3)	0.6649 (2)	0.4985 (2)	0.0509 (5)
H2	0.2297	0.7550	0.4893	0.061*
C18	0.2022 (3)	-0.0779 (2)	0.7290 (2)	0.0526 (5)
H18	0.1369	-0.0588	0.6741	0.063*
C1	0.1616 (2)	0.5591 (2)	0.42159 (18)	0.0435 (5)
C19	0.1623 (3)	-0.1735 (3)	0.8109 (3)	0.0635 (7)
H19	0.0701	-0.2179	0.8105	0.076*
C20	0.2571 (4)	-0.2044 (3)	0.8934 (3)	0.0696 (8)
C23	0.2127 (6)	-0.3092 (5)	0.9833 (4)	0.1272 (18)
H23A	0.2132	-0.2599	1.0615	0.153*
H23B	0.1177	-0.3540	0.9615	0.153*
C24	0.2878 (8)	-0.4092 (5)	0.9959 (6)	0.176 (3)
H24A	0.2747	-0.4704	0.9241	0.265*
H24B	0.2573	-0.4596	1.0633	0.265*
H24C	0.3841	-0.3678	1.0091	0.265*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0752 (2)	0.07064 (18)	0.05709 (16)	0.03362 (14)	0.00511 (12)	0.02685 (12)
O1	0.0583 (9)	0.0377 (7)	0.0422 (8)	-0.0007 (6)	-0.0080 (7)	-0.0010 (6)
O2	0.0789 (11)	0.0361 (7)	0.0330 (7)	0.0220 (7)	-0.0028 (7)	0.0050 (5)
N1	0.0537 (10)	0.0346 (8)	0.0295 (7)	0.0124 (7)	0.0001 (7)	0.0047 (6)
C6	0.0455 (11)	0.0356 (9)	0.0288 (8)	0.0079 (8)	-0.0005 (7)	0.0055 (7)
C8	0.0429 (10)	0.0304 (8)	0.0320 (8)	0.0066 (7)	0.0053 (7)	0.0049 (7)
N2	0.0735 (14)	0.0594 (12)	0.0382 (9)	0.0142 (10)	0.0083 (9)	0.0069 (8)
C7	0.0412 (10)	0.0300 (8)	0.0291 (8)	0.0052 (7)	0.0001 (7)	0.0039 (6)
C16	0.0513 (12)	0.0412 (10)	0.0350 (9)	0.0146 (9)	-0.0007 (8)	0.0062 (8)
C10	0.0436 (10)	0.0357 (9)	0.0308 (8)	0.0095 (8)	0.0011 (8)	0.0014 (7)
C12	0.0593 (13)	0.0541 (12)	0.0352 (10)	0.0124 (10)	0.0019 (9)	0.0112 (9)
C17	0.0581 (13)	0.0356 (9)	0.0366 (9)	0.0177 (9)	0.0012 (9)	0.0050 (7)
C9	0.0456 (11)	0.0371 (9)	0.0358 (9)	0.0106 (8)	0.0040 (8)	0.0054 (7)
C5	0.0453 (11)	0.0463 (11)	0.0409 (10)	0.0058 (9)	-0.0069 (9)	0.0043 (8)
C22	0.0624 (14)	0.0549 (12)	0.0409 (11)	0.0214 (11)	-0.0019 (10)	0.0099 (9)
C25	0.0541 (12)	0.0369 (9)	0.0306 (9)	0.0073 (9)	-0.0022 (8)	0.0062 (7)
C4	0.0460 (11)	0.0349 (9)	0.0349 (9)	0.0039 (8)	0.0063 (8)	0.0034 (7)

C15	0.0581 (13)	0.0408 (11)	0.0420 (11)	0.0018 (9)	0.0013 (10)	0.0070 (8)
C13	0.0632 (15)	0.0609 (14)	0.0367 (10)	0.0113 (12)	-0.0076 (10)	-0.0032 (10)
C11	0.0499 (12)	0.0375 (10)	0.0362 (9)	0.0035 (8)	0.0011 (8)	0.0049 (8)
C14	0.0661 (15)	0.0468 (12)	0.0502 (12)	-0.0016 (11)	-0.0082 (11)	-0.0059 (10)
C3	0.0578 (13)	0.0316 (9)	0.0534 (12)	0.0043 (9)	0.0090 (10)	-0.0021 (8)
C21	0.090 (2)	0.0736 (17)	0.0475 (13)	0.0376 (15)	0.0040 (13)	0.0240 (12)
C2	0.0689 (15)	0.0333 (10)	0.0554 (12)	0.0172 (10)	0.0163 (11)	0.0099 (9)
C18	0.0597 (14)	0.0463 (12)	0.0552 (13)	0.0176 (10)	0.0010 (11)	0.0091 (10)
C1	0.0510 (12)	0.0446 (11)	0.0412 (10)	0.0192 (9)	0.0118 (9)	0.0144 (8)
C19	0.0729 (17)	0.0464 (12)	0.0751 (17)	0.0147 (12)	0.0211 (14)	0.0150 (12)
C20	0.101 (2)	0.0574 (14)	0.0624 (15)	0.0338 (15)	0.0275 (15)	0.0264 (12)
C23	0.182 (5)	0.104 (3)	0.122 (3)	0.057 (3)	0.067 (3)	0.080 (3)
C24	0.283 (8)	0.101 (3)	0.174 (5)	0.071 (4)	0.070 (5)	0.086 (4)

Geometric parameters (Å, °)

Br1—C1	1.886 (2)	C5—H5B	0.9700
O1—C4	1.365 (3)	C22—C21	1.382 (3)
O1—C5	1.418 (3)	C22—H22	0.9300
O2—C16	1.426 (2)	C4—C3	1.386 (3)
O2—N1	1.467 (2)	C15—C14	1.388 (3)
N1—C10	1.435 (2)	C15—H15	0.9300
N1—C7	1.485 (2)	C13—C14	1.365 (4)
C6—C25	1.469 (3)	C13—H13	0.9300
C6—C5	1.524 (3)	C11—H11	0.9300
C6—C7	1.536 (2)	C14—H14	0.9300
C6—C16	1.569 (3)	C3—C2	1.363 (3)
C8—C9	1.389 (3)	C3—H3	0.9300
C8—C4	1.393 (3)	C21—C20	1.376 (4)
C8—C7	1.505 (2)	C21—H21	0.9300
N2—C25	1.130 (3)	C2—C1	1.384 (3)
C7—H7	0.9800	C2—H2	0.9300
C16—C17	1.495 (3)	C18—C19	1.381 (3)
C16—H16	0.9800	C18—H18	0.9300
C10—C15	1.377 (3)	C19—C20	1.382 (4)
C10—C11	1.381 (3)	C19—H19	0.9300
C12—C13	1.375 (3)	C20—C23	1.516 (4)
C12—C11	1.376 (3)	C23—C24	1.371 (6)
C12—H12	0.9300	C23—H23A	0.9700
C17—C18	1.381 (3)	C23—H23B	0.9700
C17—C22	1.382 (3)	C24—H24A	0.9600
C9—C1	1.379 (3)	C24—H24B	0.9600
C9—H9	0.9300	C24—H24C	0.9600
C5—H5A	0.9700		
C4—O1—C5	114.15 (15)	O1—C4—C3	116.29 (18)
C16—O2—N1	102.54 (13)	O1—C4—C8	122.97 (17)
C10—N1—O2	107.73 (14)	C3—C4—C8	120.7 (2)
C10—N1—C7	115.95 (15)	C10—C15—C14	119.2 (2)
O2—N1—C7	99.71 (13)	C10—C15—H15	120.4

C25—C6—C5	109.23 (16)	C14—C15—H15	120.4
C25—C6—C7	111.41 (16)	C14—C13—C12	119.8 (2)
C5—C6—C7	108.42 (15)	C14—C13—H13	120.1
C25—C6—C16	114.63 (16)	C12—C13—H13	120.1
C5—C6—C16	110.13 (17)	C12—C11—C10	120.00 (19)
C7—C6—C16	102.74 (14)	C12—C11—H11	120.0
C9—C8—C4	118.41 (17)	C10—C11—H11	120.0
C9—C8—C7	120.38 (17)	C13—C14—C15	120.8 (2)
C4—C8—C7	120.82 (17)	C13—C14—H14	119.6
N1—C7—C8	115.44 (15)	C15—C14—H14	119.6
N1—C7—C6	98.84 (14)	C2—C3—C4	120.4 (2)
C8—C7—C6	112.34 (15)	C2—C3—H3	119.8
N1—C7—H7	109.9	C4—C3—H3	119.8
C8—C7—H7	109.9	C20—C21—C22	121.5 (2)
C6—C7—H7	109.9	C20—C21—H21	119.3
O2—C16—C17	109.47 (17)	C22—C21—H21	119.3
O2—C16—C6	104.02 (15)	C3—C2—C1	119.47 (19)
C17—C16—C6	116.39 (16)	C3—C2—H2	120.3
O2—C16—H16	108.9	C1—C2—H2	120.3
C17—C16—H16	108.9	C17—C18—C19	120.5 (2)
C6—C16—H16	108.9	C17—C18—H18	119.7
C15—C10—C11	120.04 (18)	C19—C18—H18	119.7
C15—C10—N1	123.18 (17)	C9—C1—C2	120.9 (2)
C11—C10—N1	116.75 (17)	C9—C1—Br1	119.56 (16)
C13—C12—C11	120.2 (2)	C2—C1—Br1	119.56 (15)
C13—C12—H12	119.9	C18—C19—C20	121.1 (3)
C11—C12—H12	119.9	C18—C19—H19	119.5
C18—C17—C22	118.8 (2)	C20—C19—H19	119.5
C18—C17—C16	121.91 (19)	C21—C20—C19	118.0 (2)
C22—C17—C16	119.3 (2)	C21—C20—C23	121.1 (3)
C1—C9—C8	120.11 (19)	C19—C20—C23	120.9 (3)
C1—C9—H9	119.9	C24—C23—C20	118.3 (4)
C8—C9—H9	119.9	C24—C23—H23A	107.7
O1—C5—C6	111.55 (17)	C20—C23—H23A	107.7
O1—C5—H5A	109.3	C24—C23—H23B	107.7
C6—C5—H5A	109.3	C20—C23—H23B	107.7
O1—C5—H5B	109.3	H23A—C23—H23B	107.1
C6—C5—H5B	109.3	C23—C24—H24A	109.5
H5A—C5—H5B	108.0	C23—C24—H24B	109.5
C17—C22—C21	120.2 (2)	H24A—C24—H24B	109.5
C17—C22—H22	119.9	C23—C24—H24C	109.5
C21—C22—H22	119.9	H24A—C24—H24C	109.5
N2—C25—C6	177.6 (2)	H24B—C24—H24C	109.5
C16—O2—N1—C10	-176.95 (16)	C7—C6—C5—O1	62.4 (2)
C16—O2—N1—C7	-55.56 (17)	C16—C6—C5—O1	174.11 (15)
C10—N1—C7—C8	-72.5 (2)	C18—C17—C22—C21	-0.7 (3)
O2—N1—C7—C8	172.22 (15)	C16—C17—C22—C21	177.9 (2)
C10—N1—C7—C6	167.50 (15)	C5—O1—C4—C3	-162.91 (18)

O2—N1—C7—C6	52.22 (15)	C5—O1—C4—C8	19.5 (3)
C9—C8—C7—N1	80.4 (2)	C9—C8—C4—O1	178.12 (18)
C4—C8—C7—N1	-106.9 (2)	C7—C8—C4—O1	5.2 (3)
C9—C8—C7—C6	-167.34 (17)	C9—C8—C4—C3	0.7 (3)
C4—C8—C7—C6	5.4 (3)	C7—C8—C4—C3	-172.24 (18)
C25—C6—C7—N1	-154.08 (15)	C11—C10—C15—C14	1.0 (3)
C5—C6—C7—N1	85.69 (17)	N1—C10—C15—C14	-177.1 (2)
C16—C6—C7—N1	-30.87 (17)	C11—C12—C13—C14	1.2 (4)
C25—C6—C7—C8	83.6 (2)	C13—C12—C11—C10	-1.8 (3)
C5—C6—C7—C8	-36.6 (2)	C15—C10—C11—C12	0.7 (3)
C16—C6—C7—C8	-153.14 (16)	N1—C10—C11—C12	178.96 (19)
N1—O2—C16—C17	158.99 (16)	C12—C13—C14—C15	0.6 (4)
N1—O2—C16—C6	33.95 (19)	C10—C15—C14—C13	-1.7 (4)
C25—C6—C16—O2	119.69 (18)	O1—C4—C3—C2	-179.65 (19)
C5—C6—C16—O2	-116.68 (17)	C8—C4—C3—C2	-2.0 (3)
C7—C6—C16—O2	-1.34 (19)	C17—C22—C21—C20	1.0 (4)
C25—C6—C16—C17	-0.8 (3)	C4—C3—C2—C1	0.9 (3)
C5—C6—C16—C17	122.83 (19)	C22—C17—C18—C19	0.3 (3)
C7—C6—C16—C17	-121.83 (18)	C16—C17—C18—C19	-178.3 (2)
O2—N1—C10—C15	20.2 (3)	C8—C9—C1—C2	-3.0 (3)
C7—N1—C10—C15	-90.5 (2)	C8—C9—C1—Br1	177.82 (14)
O2—N1—C10—C11	-158.00 (17)	C3—C2—C1—C9	1.6 (3)
C7—N1—C10—C11	91.4 (2)	C3—C2—C1—Br1	-179.19 (17)
O2—C16—C17—C18	-47.1 (3)	C17—C18—C19—C20	-0.1 (4)
C6—C16—C17—C18	70.4 (3)	C22—C21—C20—C19	-0.9 (4)
O2—C16—C17—C22	134.4 (2)	C22—C21—C20—C23	179.7 (3)
C6—C16—C17—C22	-108.1 (2)	C18—C19—C20—C21	0.4 (4)
C4—C8—C9—C1	1.8 (3)	C18—C19—C20—C23	179.8 (3)
C7—C8—C9—C1	174.74 (17)	C21—C20—C23—C24	-49.4 (7)
C4—O1—C5—C6	-54.0 (2)	C19—C20—C23—C24	131.2 (5)
C25—C6—C5—O1	-59.2 (2)		

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

$Cg3$, $Cg4$ and $Cg5$ are the centroids of the C1–C4/C8/C9, C10–C15 and C17–C22 rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C11—H11 \cdots O1 ⁱ	0.93	2.57	3.475 (2)	165
C3—H3 \cdots $Cg5^{ii}$	0.93	2.78	3.491 (3)	134
C5—H5B \cdots $Cg3^i$	0.97	2.86	3.730 (4)	149
C22—H22 \cdots $Cg4^{iii}$	0.93	2.95	3.628 (3)	131

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