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## Structure Reports

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# Methyl 9-(4-bromophenyl)-8a,9,9a,10,-11,12,13,14a-octahydro-8H-benzo[f]-chromeno[3,4-b]indolizine-8a-carboxylate

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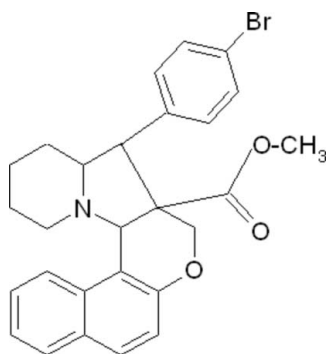
Received 18 September 2009; accepted 19 September 2009

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  $R$  factor = 0.042;  $wR$  factor = 0.108; data-to-parameter ratio = 18.4.

In the title compound,  $\text{C}_{27}\text{H}_{26}\text{BrNO}_3$ , the mean plane of the naphthalene ring system makes a dihedral angle of  $22.0$  ( $1^\circ$ ) with the bromo-substituted benzene ring. The pyrrolidine and piperidine rings exhibit envelope and chair conformations, respectively. An intermolecular  $\text{C}-\text{H}\cdots\text{Br}$  interaction is observed.

## Related literature

For the biological activity of indolizine derivatives, see: Gundersen *et al.* (2003); Teklu *et al.* (2005); Foster *et al.* (1995); Malonne *et al.* (1998); Medda *et al.* (2003). For related structures, see: Gunasekaran *et al.* (2009); Kamala *et al.* (2009).



## Experimental

### Crystal data

 $\text{C}_{27}\text{H}_{26}\text{BrNO}_3$  $M_r = 492.40$ 

Trigonal,  $P\bar{3}$   
 $a = 18.4405$  (8) Å  
 $c = 11.4828$  (8) Å  
 $V = 3381.6$  (3) Å<sup>3</sup>  
 $Z = 6$

Mo  $K\alpha$  radiation  
 $\mu = 1.85$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.25 \times 0.20 \times 0.20$  mm

### Data collection

Bruker Kappa APEXII CCD diffractometer  
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.654$ ,  $T_{\max} = 0.708$

23085 measured reflections  
5338 independent reflections  
2509 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.113$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$   
 $wR(F^2) = 0.108$   
 $S = 0.85$   
5338 reflections  
290 parameters

2 restraints  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.85$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.33$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C}15-\text{H}15\text{B}\cdots\text{Br}1^i$	0.97	2.73	3.588 (3)	147

Symmetry code: (i)  $-x + y + 1, -x + 1, z - 1$ .

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); 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.

BG thanks AMET University management, India, for their kind support. BG also acknowledges SAIF, IIT Madras, India, for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2463).

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## supporting information

*Acta Cryst.* (2009). E65, o2550 [doi:10.1107/S1600536809037994]

## Methyl 9-(4-bromophenyl)-8a,9,9a,10,11,12,13,14a-octahydro-8H-benzo[*f*]chromeno[3,4-*b*]indolizine-8a-carboxylate

B. Gunasekaran, S. Kathiravan, R. Raghunathan, G. Chakkaravarthi and V. Manivannan

### S1. Comment

Indolizine derivatives exhibit antioxidative (Teklu *et al.*, 2005), antiherpes (Foster *et al.*, 1995), anti-inflammatory (Malonne *et al.*, 1998) and antiviral (Medda *et al.*, 2003) activities. In addition, indolizines are used as antimycobacterial agents against mycobacterial tuberculosis (Gundersen *et al.*, 2003).

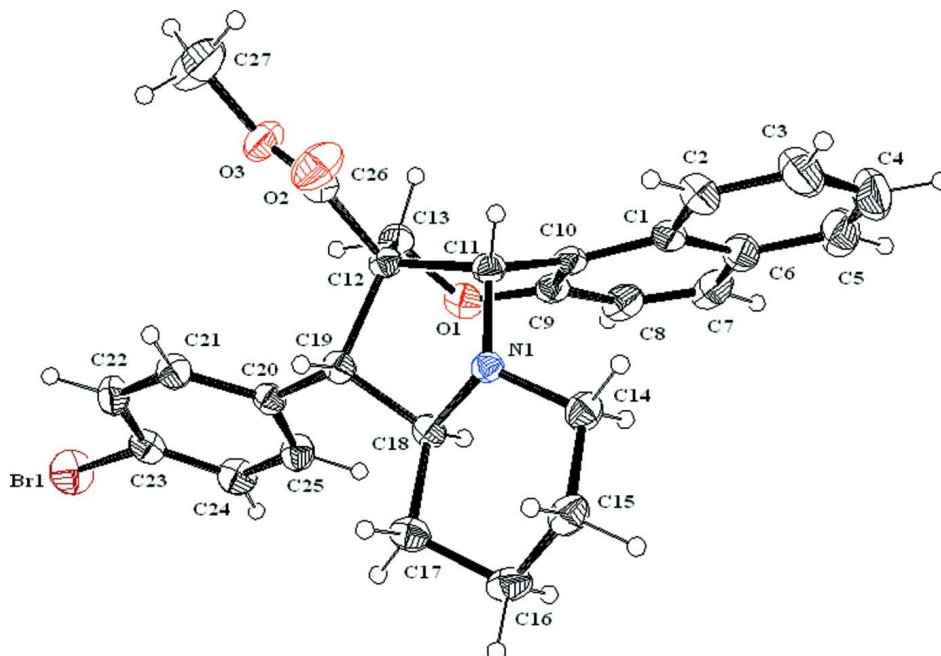
The geometric parameters of the title compound (Fig. 1) agree well with reported similar structures (Gunasekaran *et al.*, 2009; Kamala *et al.*, 2009). The mean plane of naphthalene ring makes the dihedral angle of 22.0 (1)° with the benzene ring. The pyrrolidine ring exhibits an envelope conformation and the piperidine (N1/C14–C18) ring exhibits a chair conformation [C16—C15—C14—N1 = 56.3 (3)° and C16—C17—C18—N1 = -53.9 (3)°]. The sum of bond angles around N1 [338.3 (2)°] indicates *sp*<sup>3</sup> hybridization.

### S2. Experimental

A mixture of (*Z*)-methyl 2-((1-formylnaphthalen-2-yloxy)methyl)-3-(4-bromophenyl)acrylate (20 mmol) and piperidine-2-carboxylic acid (30 mmol) were refluxed in benzene for 20 h and the solvent was removed under reduced pressure. The crude product was subjected to column chromatography to get the pure product. Chloroform and methanol (1:1) solvent mixture was used for the crystallization under slow evaporation method.

### S3. Refinement

H atoms were positioned geometrically and refined using riding model with C—H = 0.93 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for aromatic C—H, C—H = 0.98 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for CH, C—H = 0.97 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for CH<sub>2</sub>, and C—H = 0.96 Å and  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$  for CH<sub>3</sub>. The components of the anisotropic displacement parameters in direction of the bond of C1, C2, C26 and O2 were restrained to be equal within an effective standard deviation of 0.001 using the DELU command in *SHELXL* (Sheldrick, 2008).

**Figure 1**

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

**Methyl 9-(4-bromophenyl)-8a,9,9a,10,11,12,13,14a-octahydro-8H- benzo[f]chromeno[3,4-b]indolizine-8a-carboxylate**

*Crystal data*

$C_{27}H_{26}BrNO_3$

$M_r = 492.40$

Trigonal,  $P\bar{3}$

Hall symbol: -P 3

$a = 18.4405 (8) \text{ \AA}$

$c = 11.4828 (8) \text{ \AA}$

$V = 3381.6 (3) \text{ \AA}^3$

$Z = 6$

$F(000) = 1524$

$D_x = 1.451 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 4759 reflections

$\theta = 2.2\text{--}25.7^\circ$

$\mu = 1.85 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Block, colourless

$0.25 \times 0.20 \times 0.20 \text{ mm}$

*Data collection*

Bruker Kappa APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 0 pixels  $\text{mm}^{-1}$

$\omega$  and  $\varphi$  scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.654$ ,  $T_{\max} = 0.708$

23085 measured reflections

5338 independent reflections

2509 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.113$

$\theta_{\max} = 27.8^\circ$ ,  $\theta_{\min} = 2.2^\circ$

$h = -22 \rightarrow 24$

$k = -24 \rightarrow 24$

$l = -8 \rightarrow 15$

Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.042$

$wR(F^2) = 0.108$

$S = 0.85$

5338 reflections

290 parameters

2 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

$w = 1/[\sigma^2(F_o^2) + (0.0452P)^2]$

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

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

$\Delta\rho_{\max} = 0.85 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.33 \text{ e } \text{\AA}^{-3}$

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.32587 (18)	0.03952 (17)	-0.2836 (3)	0.0450 (7)
C2	0.2679 (2)	0.0537 (2)	-0.3441 (3)	0.0616 (9)
H2	0.2401	0.0769	-0.3050	0.074*
C3	0.2515 (3)	0.0339 (2)	-0.4604 (3)	0.0850 (13)
H3	0.2123	0.0432	-0.4982	0.102*
C4	0.2927 (3)	0.0004 (2)	-0.5221 (3)	0.0859 (13)
H4	0.2821	-0.0115	-0.6011	0.103*
C5	0.3479 (3)	-0.0149 (2)	-0.4667 (3)	0.0786 (12)
H5	0.3752	-0.0375	-0.5082	0.094*
C6	0.3654 (2)	0.00269 (18)	-0.3465 (3)	0.0564 (9)
C7	0.4228 (2)	-0.01415 (18)	-0.2873 (3)	0.0627 (10)
H7	0.4519	-0.0349	-0.3286	0.075*
C8	0.43567 (19)	-0.00053 (17)	-0.1725 (3)	0.0513 (8)
H8	0.4704	-0.0156	-0.1336	0.062*
C9	0.39688 (17)	0.03636 (16)	-0.1111 (2)	0.0384 (7)
C10	0.34630 (16)	0.06057 (15)	-0.1639 (2)	0.0356 (7)
C11	0.32309 (16)	0.11839 (16)	-0.1002 (2)	0.0341 (6)
H11	0.2669	0.1056	-0.1242	0.041*
C12	0.32533 (15)	0.11112 (16)	0.0348 (2)	0.0333 (6)
C13	0.34153 (18)	0.04079 (17)	0.0692 (2)	0.0431 (7)
H13A	0.3526	0.0438	0.1522	0.052*
H13B	0.2920	-0.0127	0.0531	0.052*
C14	0.41242 (18)	0.23382 (17)	-0.2399 (2)	0.0434 (7)
H14A	0.3650	0.2180	-0.2912	0.052*
H14B	0.4416	0.2053	-0.2663	0.052*
C15	0.47016 (18)	0.32660 (18)	-0.2460 (2)	0.0477 (8)
H15A	0.4395	0.3550	-0.2268	0.057*
H15B	0.4914	0.3422	-0.3247	0.057*
C16	0.54293 (18)	0.35396 (18)	-0.1621 (3)	0.0492 (8)
H16A	0.5765	0.3293	-0.1850	0.059*
H16B	0.5782	0.4144	-0.1644	0.059*
C17	0.50984 (18)	0.32634 (16)	-0.0398 (2)	0.0425 (7)
H17A	0.5562	0.3404	0.0128	0.051*
H17B	0.4815	0.3558	-0.0140	0.051*

C18	0.44950 (16)	0.23290 (15)	-0.0361 (2)	0.0329 (6)
H18	0.4799	0.2029	-0.0508	0.039*
C19	0.39796 (15)	0.19968 (16)	0.0742 (2)	0.0323 (6)
H19	0.3722	0.2342	0.0882	0.039*
C20	0.44263 (16)	0.20142 (16)	0.1853 (2)	0.0326 (6)
C21	0.40965 (17)	0.20588 (17)	0.2912 (2)	0.0395 (7)
H21	0.3612	0.2096	0.2925	0.047*
C22	0.44673 (19)	0.20491 (18)	0.3956 (2)	0.0454 (8)
H22	0.4232	0.2072	0.4662	0.054*
C23	0.51857 (18)	0.20047 (17)	0.3933 (2)	0.0414 (7)
C24	0.55532 (18)	0.19869 (17)	0.2895 (3)	0.0461 (8)
H24	0.6053	0.1979	0.2888	0.055*
C25	0.51612 (17)	0.19814 (17)	0.1866 (2)	0.0426 (7)
H25	0.5397	0.1955	0.1162	0.051*
C26	0.24417 (18)	0.09807 (19)	0.0883 (3)	0.0456 (7)
C27	0.1435 (2)	0.0356 (3)	0.2332 (4)	0.0985 (14)
H27A	0.1533	0.0860	0.2714	0.148*
H27B	0.1240	-0.0091	0.2891	0.148*
H27C	0.1021	0.0211	0.1735	0.148*
N1	0.38286 (13)	0.20806 (12)	-0.12185 (17)	0.0301 (5)
O1	0.41141 (11)	0.04609 (11)	0.00670 (17)	0.0446 (5)
O2	0.20524 (13)	0.12926 (15)	0.0531 (2)	0.0685 (7)
O3	0.22148 (12)	0.04877 (13)	0.18093 (17)	0.0569 (6)
Br1	0.56763 (2)	0.19502 (2)	0.53512 (3)	0.06620 (16)

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0421 (18)	0.0299 (16)	0.0472 (19)	0.0063 (14)	0.0072 (13)	-0.0069 (14)
C2	0.056 (2)	0.060 (2)	0.052 (2)	0.0171 (17)	-0.0091 (16)	-0.0117 (17)
C3	0.091 (3)	0.073 (3)	0.059 (3)	0.016 (2)	-0.019 (2)	-0.012 (2)
C4	0.116 (4)	0.060 (3)	0.052 (3)	0.021 (3)	0.002 (3)	-0.016 (2)
C5	0.110 (3)	0.042 (2)	0.061 (3)	0.022 (2)	0.020 (2)	-0.0113 (19)
C6	0.070 (2)	0.0282 (18)	0.053 (2)	0.0107 (17)	0.0124 (18)	-0.0059 (15)
C7	0.074 (3)	0.0336 (19)	0.077 (3)	0.0245 (19)	0.036 (2)	0.0021 (18)
C8	0.056 (2)	0.0335 (18)	0.068 (2)	0.0251 (16)	0.0165 (18)	0.0085 (16)
C9	0.0382 (17)	0.0246 (15)	0.0459 (19)	0.0109 (14)	0.0076 (14)	0.0020 (13)
C10	0.0324 (16)	0.0240 (15)	0.0413 (17)	0.0071 (13)	0.0047 (13)	-0.0016 (12)
C11	0.0281 (15)	0.0342 (16)	0.0382 (16)	0.0142 (13)	-0.0002 (12)	-0.0010 (13)
C12	0.0313 (16)	0.0295 (15)	0.0368 (16)	0.0134 (13)	0.0027 (12)	0.0023 (12)
C13	0.0474 (19)	0.0340 (17)	0.0440 (17)	0.0175 (15)	0.0040 (14)	0.0025 (13)
C14	0.0450 (18)	0.0462 (19)	0.0402 (17)	0.0236 (16)	0.0022 (14)	0.0055 (14)
C15	0.051 (2)	0.046 (2)	0.0464 (18)	0.0243 (16)	0.0104 (15)	0.0115 (15)
C16	0.0425 (18)	0.0320 (17)	0.069 (2)	0.0157 (15)	0.0108 (16)	0.0068 (15)
C17	0.0395 (18)	0.0322 (16)	0.0538 (19)	0.0165 (14)	-0.0031 (14)	-0.0018 (14)
C18	0.0354 (16)	0.0291 (15)	0.0369 (15)	0.0182 (13)	-0.0024 (13)	-0.0020 (12)
C19	0.0321 (16)	0.0315 (15)	0.0383 (16)	0.0197 (13)	-0.0019 (12)	-0.0035 (12)
C20	0.0346 (16)	0.0288 (15)	0.0370 (16)	0.0178 (13)	-0.0026 (12)	-0.0039 (12)

C21	0.0344 (16)	0.0452 (18)	0.0452 (18)	0.0246 (15)	-0.0037 (14)	-0.0045 (14)
C22	0.050 (2)	0.055 (2)	0.0356 (17)	0.0298 (17)	-0.0023 (14)	-0.0059 (14)
C23	0.0450 (19)	0.0389 (18)	0.0412 (18)	0.0217 (15)	-0.0112 (14)	0.0008 (13)
C24	0.0398 (18)	0.0508 (19)	0.056 (2)	0.0286 (16)	-0.0092 (15)	-0.0005 (15)
C25	0.0427 (18)	0.0492 (19)	0.0432 (18)	0.0285 (15)	-0.0001 (14)	-0.0020 (14)
C26	0.0377 (18)	0.0465 (19)	0.0462 (19)	0.0162 (14)	0.0011 (14)	-0.0031 (15)
C27	0.079 (3)	0.108 (3)	0.103 (3)	0.043 (3)	0.044 (2)	0.021 (3)
N1	0.0292 (12)	0.0280 (12)	0.0332 (12)	0.0143 (10)	0.0022 (10)	0.0007 (10)
O1	0.0462 (13)	0.0353 (12)	0.0571 (14)	0.0238 (10)	-0.0026 (10)	-0.0004 (10)
O2	0.0512 (15)	0.0940 (19)	0.0727 (16)	0.0455 (13)	0.0179 (12)	0.0238 (13)
O3	0.0493 (14)	0.0684 (15)	0.0484 (13)	0.0260 (12)	0.0151 (10)	0.0127 (11)
Br1	0.0694 (3)	0.0800 (3)	0.0538 (2)	0.0408 (2)	-0.01750 (18)	0.00658 (18)

*Geometric parameters (Å, °)*

C1—C2	1.406 (4)	C15—C16	1.518 (4)
C1—C6	1.417 (4)	C15—H15A	0.9700
C1—C10	1.427 (4)	C15—H15B	0.9700
C2—C3	1.377 (4)	C16—C17	1.515 (4)
C2—H2	0.9300	C16—H16A	0.9700
C3—C4	1.390 (6)	C16—H16B	0.9700
C3—H3	0.9300	C17—C18	1.514 (4)
C4—C5	1.344 (5)	C17—H17A	0.9700
C4—H4	0.9300	C17—H17B	0.9700
C5—C6	1.418 (5)	C18—N1	1.459 (3)
C5—H5	0.9300	C18—C19	1.516 (3)
C6—C7	1.416 (5)	C18—H18	0.9800
C7—C8	1.341 (4)	C19—C20	1.511 (3)
C7—H7	0.9300	C19—H19	0.9800
C8—C9	1.399 (4)	C20—C21	1.380 (3)
C8—H8	0.9300	C20—C25	1.387 (4)
C9—C10	1.361 (4)	C21—C22	1.385 (4)
C9—O1	1.374 (3)	C21—H21	0.9300
C10—C11	1.521 (4)	C22—C23	1.368 (4)
C11—N1	1.479 (3)	C22—H22	0.9300
C11—C12	1.558 (3)	C23—C24	1.379 (4)
C11—H11	0.9800	C23—Br1	1.890 (3)
C12—C26	1.521 (4)	C24—C25	1.383 (4)
C12—C13	1.521 (4)	C24—H24	0.9300
C12—C19	1.574 (3)	C25—H25	0.9300
C13—O1	1.435 (3)	C26—O2	1.193 (3)
C13—H13A	0.9700	C26—O3	1.324 (3)
C13—H13B	0.9700	C27—O3	1.461 (4)
C14—N1	1.450 (3)	C27—H27A	0.9600
C14—C15	1.498 (4)	C27—H27B	0.9600
C14—H14A	0.9700	C27—H27C	0.9600
C14—H14B	0.9700		

C2—C1—C6	117.4 (3)	C16—C15—H15B	109.5
C2—C1—C10	123.2 (3)	H15A—C15—H15B	108.1
C6—C1—C10	119.4 (3)	C17—C16—C15	109.6 (2)
C3—C2—C1	121.0 (3)	C17—C16—H16A	109.7
C3—C2—H2	119.5	C15—C16—H16A	109.7
C1—C2—H2	119.5	C17—C16—H16B	109.7
C2—C3—C4	121.1 (4)	C15—C16—H16B	109.7
C2—C3—H3	119.4	H16A—C16—H16B	108.2
C4—C3—H3	119.4	C18—C17—C16	110.6 (2)
C5—C4—C3	119.4 (4)	C18—C17—H17A	109.5
C5—C4—H4	120.3	C16—C17—H17A	109.5
C3—C4—H4	120.3	C18—C17—H17B	109.5
C4—C5—C6	121.5 (4)	C16—C17—H17B	109.5
C4—C5—H5	119.2	H17A—C17—H17B	108.1
C6—C5—H5	119.2	N1—C18—C17	111.3 (2)
C7—C6—C1	118.7 (3)	N1—C18—C19	100.2 (2)
C7—C6—C5	121.8 (3)	C17—C18—C19	116.0 (2)
C1—C6—C5	119.5 (4)	N1—C18—H18	109.6
C8—C7—C6	120.8 (3)	C17—C18—H18	109.6
C8—C7—H7	119.6	C19—C18—H18	109.6
C6—C7—H7	119.6	C20—C19—C18	118.2 (2)
C7—C8—C9	120.0 (3)	C20—C19—C12	115.9 (2)
C7—C8—H8	120.0	C18—C19—C12	102.47 (19)
C9—C8—H8	120.0	C20—C19—H19	106.5
C10—C9—O1	121.1 (2)	C18—C19—H19	106.5
C10—C9—C8	122.4 (3)	C12—C19—H19	106.5
O1—C9—C8	116.5 (3)	C21—C20—C25	117.6 (2)
C9—C10—C1	118.1 (3)	C21—C20—C19	119.6 (2)
C9—C10—C11	119.7 (2)	C25—C20—C19	122.8 (2)
C1—C10—C11	121.7 (3)	C20—C21—C22	121.8 (3)
N1—C11—C10	112.9 (2)	C20—C21—H21	119.1
N1—C11—C12	103.10 (19)	C22—C21—H21	119.1
C10—C11—C12	112.9 (2)	C23—C22—C21	118.9 (3)
N1—C11—H11	109.2	C23—C22—H22	120.6
C10—C11—H11	109.2	C21—C22—H22	120.6
C12—C11—H11	109.2	C22—C23—C24	121.4 (2)
C26—C12—C13	111.0 (2)	C22—C23—Br1	119.3 (2)
C26—C12—C11	110.4 (2)	C24—C23—Br1	119.3 (2)
C13—C12—C11	110.9 (2)	C23—C24—C25	118.5 (3)
C26—C12—C19	107.9 (2)	C23—C24—H24	120.7
C13—C12—C19	112.5 (2)	C25—C24—H24	120.7
C11—C12—C19	103.98 (19)	C24—C25—C20	121.8 (3)
O1—C13—C12	111.4 (2)	C24—C25—H25	119.1
O1—C13—H13A	109.3	C20—C25—H25	119.1
C12—C13—H13A	109.3	O2—C26—O3	122.9 (3)
O1—C13—H13B	109.3	O2—C26—C12	124.7 (3)
C12—C13—H13B	109.3	O3—C26—C12	112.4 (3)
H13A—C13—H13B	108.0	O3—C27—H27A	109.5

N1—C14—C15	110.7 (2)	O3—C27—H27B	109.5
N1—C14—H14A	109.5	H27A—C27—H27B	109.5
C15—C14—H14A	109.5	O3—C27—H27C	109.5
N1—C14—H14B	109.5	H27A—C27—H27C	109.5
C15—C14—H14B	109.5	H27B—C27—H27C	109.5
H14A—C14—H14B	108.1	C14—N1—C18	114.1 (2)
C14—C15—C16	110.8 (2)	C14—N1—C11	118.1 (2)
C14—C15—H15A	109.5	C18—N1—C11	106.10 (18)
C16—C15—H15A	109.5	C9—O1—C13	112.0 (2)
C14—C15—H15B	109.5	C26—O3—C27	113.0 (3)
C6—C1—C2—C3	-1.2 (5)	N1—C18—C19—C12	42.9 (2)
C10—C1—C2—C3	178.6 (3)	C17—C18—C19—C12	162.8 (2)
C1—C2—C3—C4	-0.9 (6)	C26—C12—C19—C20	90.7 (3)
C2—C3—C4—C5	1.6 (6)	C13—C12—C19—C20	-32.0 (3)
C3—C4—C5—C6	-0.1 (6)	C11—C12—C19—C20	-152.0 (2)
C2—C1—C6—C7	-178.6 (3)	C26—C12—C19—C18	-139.1 (2)
C10—C1—C6—C7	1.6 (4)	C13—C12—C19—C18	98.1 (2)
C2—C1—C6—C5	2.5 (4)	C11—C12—C19—C18	-21.9 (2)
C10—C1—C6—C5	-177.3 (3)	C18—C19—C20—C21	153.2 (2)
C4—C5—C6—C7	179.2 (3)	C12—C19—C20—C21	-84.7 (3)
C4—C5—C6—C1	-1.9 (5)	C18—C19—C20—C25	-27.3 (4)
C1—C6—C7—C8	4.1 (5)	C12—C19—C20—C25	94.9 (3)
C5—C6—C7—C8	-177.0 (3)	C25—C20—C21—C22	-1.7 (4)
C6—C7—C8—C9	-4.6 (5)	C19—C20—C21—C22	177.9 (3)
C7—C8—C9—C10	-0.8 (4)	C20—C21—C22—C23	0.8 (4)
C7—C8—C9—O1	178.3 (3)	C21—C22—C23—C24	1.3 (4)
O1—C9—C10—C1	-172.6 (2)	C21—C22—C23—Br1	-177.7 (2)
C8—C9—C10—C1	6.5 (4)	C22—C23—C24—C25	-2.5 (4)
O1—C9—C10—C11	15.6 (4)	Br1—C23—C24—C25	176.5 (2)
C8—C9—C10—C11	-165.3 (2)	C23—C24—C25—C20	1.6 (4)
C2—C1—C10—C9	173.5 (3)	C21—C20—C25—C24	0.4 (4)
C6—C1—C10—C9	-6.7 (4)	C19—C20—C25—C24	-179.1 (2)
C2—C1—C10—C11	-14.9 (4)	C13—C12—C26—O2	-159.1 (3)
C6—C1—C10—C11	164.9 (3)	C11—C12—C26—O2	-35.8 (4)
C9—C10—C11—N1	89.9 (3)	C19—C12—C26—O2	77.2 (3)
C1—C10—C11—N1	-81.6 (3)	C13—C12—C26—O3	22.0 (3)
C9—C10—C11—C12	-26.5 (3)	C11—C12—C26—O3	145.3 (2)
C1—C10—C11—C12	162.0 (2)	C19—C12—C26—O3	-101.6 (3)
N1—C11—C12—C26	108.5 (2)	C15—C14—N1—C18	-55.9 (3)
C10—C11—C12—C26	-129.3 (2)	C15—C14—N1—C11	178.3 (2)
N1—C11—C12—C13	-128.1 (2)	C17—C18—N1—C14	54.8 (3)
C10—C11—C12—C13	-6.0 (3)	C19—C18—N1—C14	178.1 (2)
N1—C11—C12—C19	-7.0 (2)	C17—C18—N1—C11	-173.3 (2)
C10—C11—C12—C19	115.1 (2)	C19—C18—N1—C11	-50.0 (2)
C26—C12—C13—O1	172.0 (2)	C10—C11—N1—C14	42.9 (3)
C11—C12—C13—O1	48.9 (3)	C12—C11—N1—C14	165.0 (2)
C19—C12—C13—O1	-67.0 (3)	C10—C11—N1—C18	-86.7 (2)



N1—C14—C15—C16	56.3 (3)	C12—C11—N1—C18	35.5 (2)
C14—C15—C16—C17	-56.7 (3)	C10—C9—O1—C13	30.1 (3)
C15—C16—C17—C18	55.2 (3)	C8—C9—O1—C13	-149.1 (2)
C16—C17—C18—N1	-53.9 (3)	C12—C13—O1—C9	-63.2 (3)
C16—C17—C18—C19	-167.6 (2)	O2—C26—O3—C27	1.2 (4)
N1—C18—C19—C20	171.6 (2)	C12—C26—O3—C27	-180.0 (3)
C17—C18—C19—C20	-68.5 (3)		

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
C15—H15B $\cdots$ Br1 <sup>i</sup>	0.97	2.73	3.588 (3)	147

Symmetry code: (i)  $-x+y+1, -x+1, z-1$ .