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Methyl 1-benzyl-5-methyl-2,4-diphenyl-1*H*-pyrrole-3-carboxylate

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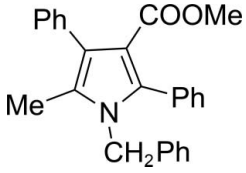
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.004 Å; R factor = 0.044; wR factor = 0.119; data-to-parameter ratio = 15.1.

In the title compound, $C_{26}H_{23}NO_2$, the dihedral angles between the pyrrole ring and the two phenyl rings are 58.1 (6) and 71.5 (5)°. The mean planes of the 5-methylbenzene ring and the carboxyl group are twisted by 89.5 (3) and 22.1 (9)°, respectively, from the pyrrole ring. In the crystal, weak C—H···O interactions lead to supramolecular layers in the *ab* plane.

Related literature

For previous münchnone-based approaches to atorvastatin, see: Pandey & Rao (2004); Park *et al.* (2008); Roth *et al.* (1991). For other examples of the synthesis of pyrroles *via* 1,3-dipolar cycloadditions with münchnones, see: Lopchuk & Gribble (2011*a*,*b*); Lopchuk *et al.* (2013). For related crystal structures, see: Grassi *et al.* (2002); Fang *et al.* (2012); Donohoe *et al.* (2010); Sun *et al.* (2004); Zhang *et al.* (2011).



Experimental

Crystal data

$C_{26}H_{23}NO_2$
M_r = 381.45
Orthorhombic, $P2_12_12_1$
a = 8.8056 (2) Å
b = 10.6638 (2) Å
c = 21.8315 (5) Å
V = 2050.00 (8) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 0.61 mm^{-1}
T = 173 K
0.28 × 0.22 × 0.12 mm

Data collection

Agilent Xcalibur (Eos Gemini) diffractometer
Absorption correction: multi-scan (*CrysAlis PRO* and *CrysAlis RED*; Agilent, 2012)
T_{min} = 0.720, T_{max} = 1.000
12873 measured reflections
3991 independent reflections
3525 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.119
S = 1.06
3991 reflections
264 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Absolute structure: Flack parameter determined using 1348 quotients (Parsons *et al.*, 2013)
Absolute structure parameter: 0.02 (18)

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

D—H···A	D—H	H···A	D···A	D—H···A
C17—H17B···O1^{i}	0.99	2.56	3.177 (3)	120
C26—H26A···O2^{ii}	0.98	2.59	3.383 (3)	138

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

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Agilent, 2012); program(s) used to solve structure: *SUPERFLIP* (Palatinus *et al.*, 2012); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2*.

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Supporting information for this paper is available from the IUCr electronic archives (Reference: TK5295).

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supplementary materials

Acta Cryst. (2014). E**70**, o338–o339 [doi:10.1107/S1600536814003316]

Methyl 1-benzyl-5-methyl-2,4-diphenyl-1*H*-pyrrole-3-carboxylate

Justin M. Lopchuk, Gordon W. Gribble and Jerry P. Jasinski

1. Chemical context

2. Structural commentary

During the course of our studies toward a total synthesis of atorvastatin, methyl 1-benzyl-5-methyl-2,4-diphenyl-1*H*-pyrrole-3-carboxylate (I), a pentasubstituted pyrrole, was generated from the reaction of a münchnone with methyl 3-phenylpropiolate. Previously published work on münchnone-based routes toward atorvastatin found that the key münchnone cycloadditions were either low yielding or unselective and delivered 1:1 mixtures of regioisomers (Pandey *et al.*, 2004; Park *et al.*, 2008; Roth *et al.*, 1991). However, our recent studies on the 1,3-dipolar cycloaddition of münchnones showed that high regioselectivies can be obtained by proper selection and combination of the münchnone, dipolarophile, and solvent (Lopchuk *et al.*, 2011*a*, Lopchuk *et al.*, 2011*b*; Lopchuk *et al.*, 2013).

A variety of related highly substituted pyrrole crystal structures have been reported including *N*-((2-methyl-4,5-diphenyl-1*H*-pyrrole-3-carbonyl)oxy)benzamide (Grassi *et al.*, 2002), *N*,1,5-tribenzyl-4-(2-chlorophenyl)-2-methyl-1*H*-pyrrole-3-carbothioamide (Fang *et al.*, 2012), 1-(2-benzyl-5-isopropyl-4-phenyl-1*H*-pyrrol-3-yl)-2-methylpropan-1-one (Sun *et al.*, 2004), 5-(4-fluorophenyl)-2-isopropyl-*N*,4-diphenyl-1*H*-pyrrole-3-carboxamide (Donohoe *et al.*, 2010), and 1-(2-benzoyl-5-isopropyl-4-phenyl-1*H*-pyrrol-3-yl)-2-methylpropan-1-one (Zhang *et al.*, 2011). In continuation of our work on münchnone-based routes this paper reports the crystal structure of the title compound, (I), $C_{26}H_{23}NO_2$,

In (I), the dihedral angles between the mean planes of the two phenyl rings (C5–C10 and C11–C16) with that of the pyrrole ring (N1/C1–C4) are 58.1 (6) and 71.5 (5)°, respectively (Fig. 1). The mean planes of the 5-methyl benzene ring (C18–C23) and carboxyl group (O1/O2/C24/C25) are also twisted by 89.5 (3) and 22.1 (9)°, respectively, from that of the pyrrole ring. In the crystal, while no classical hydrogen bonds are observed, weak C—H···O intermolecular interactions are observed (Table 1) which lead to supramolecular layers in the *ab* plane.

3. Supramolecular features

4. Database survey

5. Synthesis and crystallization

A round bottom flask was charged with *N*-benzoyl-*N*-benzylalanine (424 mg, 1.5 mmol), methyl 3-phenylpropiolate (80 mg, 0.5 mmol), and dry THF (20 ml). The reaction was placed under nitrogen and *N*,*N*′-diisopropylcarbodiimide (234 ml, 1.5 mmol) added at room temperature. The mixture was heated to reflux for 24 h (Fig. 2). The reaction was cooled to room temperature and concentrated *in vacuo*. The residue was directly purified by flash chromatography to afford pyrrole I as a clear, colorless oil which solidified upon standing (158 mg, 83%). Pyrrole I was obtained as the major isomer (96:4 ratio of I:II). Single crystals suitable for diffraction were grown from dichloromethane (slow evaporation) at ambient temperature [M.pt. 454- 455 K].

6. Refinement

All of the H atoms were placed in their calculated positions and then refined using the riding model with atom—H lengths of 0.95 Å (CH), 0.99 Å (CH_2) or 0.98 Å (CH_3). Isotropic displacement parameters for these atoms were set to 1.2 (CH, CH_2) or 1.5 (CH_3) times U_{eq} of the parent atom. Idealized methyl groups were refined as rotating.

Computing details

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO* (Agilent, 2012); data reduction: *CrysAlis RED* (Agilent, 2012); program(s) used to solve structure: SUPERFLIP (Palatinus *et al.*, 2012); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: OLEX2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: OLEX2 (Dolomanov *et al.*, 2009).

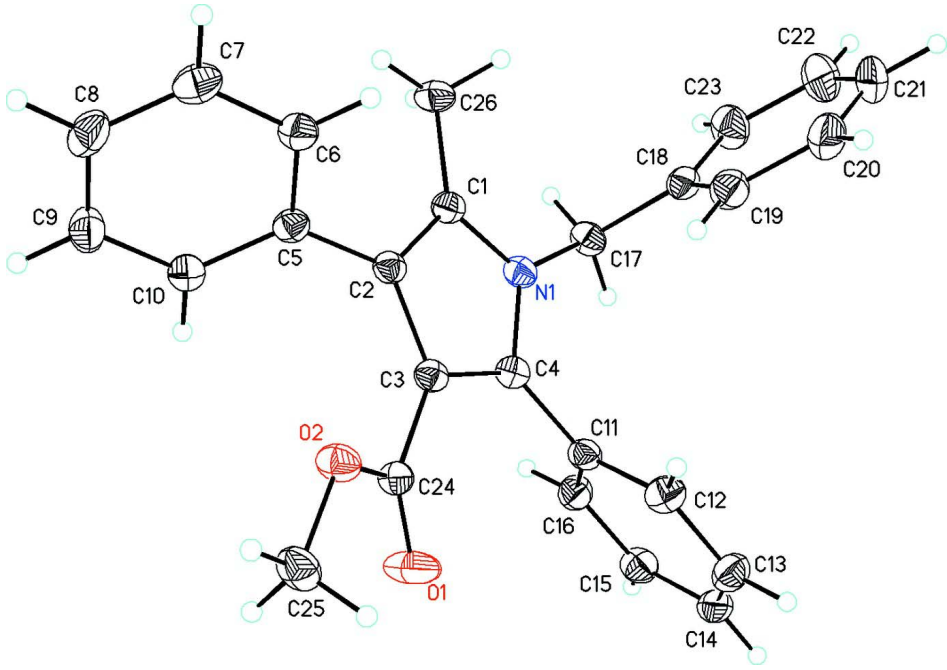

Figure 1

ORTEP drawing of (I), $C_{26}H_{23}NO_2$, showing the labeling scheme with 30% probability displacement ellipsoids.

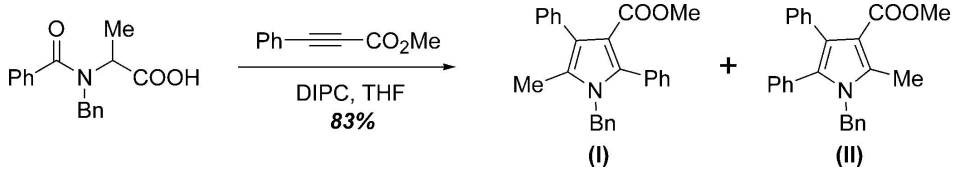

Figure 2

Reaction scheme for $C_{26}H_{23}NO_2$.

Methyl 1-benzyl-5-methyl-2,4-diphenyl-1*H*-pyrrole-3-carboxylate

Crystal data

$C_{26}H_{23}NO_2$
M_r = 381.45
Orthorhombic, $P2_12_12_1$
a = 8.8056 (2) Å
b = 10.6638 (2) Å
c = 21.8315 (5) Å
V = 2050.00 (8) Å^3
Z = 4

$F(000) = 808$
$D_x = 1.236$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.5418$ Å
Cell parameters from 4659 reflections
$\theta = 4.1–72.4°$

$\mu = 0.61$ mm^{-1}
$T = 173$ K
Irregular, colourless
0.28 × 0.22 × 0.12 mm

Data collection

Agilent Xcalibur (Eos Gemini) diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 16.0416 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO* and *CrysAlis RED*; Agilent, 2012)

$T_{min} = 0.720$, $T_{max} = 1.000$
12873 measured reflections
3991 independent reflections
3525 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$
$\theta_{max} = 72.6°$, $\theta_{min} = 4.1°$
$h = -10 \rightarrow 10$
$k = -13 \rightarrow 11$
$l = -26 \rightarrow 26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.119$
$S = 1.06$
3991 reflections
264 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0691P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}
Absolute structure: Flack parameter determined using 1348 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.02 (18)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.9445 (2)	0.4206 (2)	0.84521 (12)	0.0598 (7)
O2	0.7077 (2)	0.43820 (19)	0.87973 (9)	0.0393 (5)
N1	0.7361 (2)	0.1689 (2)	0.72021 (10)	0.0315 (5)
C1	0.6106 (3)	0.1444 (2)	0.75598 (12)	0.0309 (5)
C2	0.6162 (3)	0.2209 (2)	0.80673 (12)	0.0286 (5)
C3	0.7518 (3)	0.2943 (2)	0.80125 (11)	0.0288 (5)
C4	0.8227 (3)	0.2603 (2)	0.74693 (12)	0.0310 (6)
C5	0.5074 (3)	0.2152 (2)	0.85815 (12)	0.0307 (5)
C6	0.3528 (3)	0.2348 (3)	0.84848 (13)	0.0366 (6)
H6	0.3174	0.2554	0.8086	0.044*
C7	0.2498 (3)	0.2246 (3)	0.89631 (15)	0.0451 (7)
H7	0.1448	0.2385	0.8890	0.054*
C8	0.2991 (4)	0.1945 (3)	0.95452 (15)	0.0467 (7)
H8	0.2284	0.1861	0.9871	0.056*

C9	0.4528 (4)	0.1765 (3)	0.96491 (14)	0.0458 (7)
H9	0.4876	0.1573	1.0050	0.055*
C10	0.5561 (3)	0.1864 (3)	0.91732 (13)	0.0369 (6)
H10	0.6611	0.1734	0.9250	0.044*
C11	0.9580 (3)	0.3149 (2)	0.71660 (11)	0.0319 (6)
C12	0.9505 (3)	0.4354 (3)	0.69197 (14)	0.0402 (6)
H12	0.8580	0.4811	0.6938	0.048*
C13	1.0765 (4)	0.4889 (3)	0.66490 (15)	0.0437 (7)
H13	1.0706	0.5715	0.6488	0.052*
C14	1.2107 (3)	0.4232 (3)	0.66111 (13)	0.0413 (7)
H14	1.2972	0.4604	0.6425	0.050*
C15	1.2193 (3)	0.3033 (3)	0.68443 (14)	0.0419 (7)
H15	1.3114	0.2573	0.6813	0.050*
C16	1.0935 (3)	0.2494 (3)	0.71249 (14)	0.0386 (6)
H16	1.1005	0.1672	0.7290	0.046*
C17	0.7718 (3)	0.1039 (3)	0.66289 (12)	0.0355 (6)
H17A	0.7508	0.0134	0.6684	0.043*
H17B	0.8818	0.1131	0.6546	0.043*
C18	0.6847 (3)	0.1500 (3)	0.60767 (13)	0.0357 (6)
C19	0.6183 (4)	0.2672 (3)	0.60486 (15)	0.0450 (7)
H19	0.6225	0.3213	0.6394	0.054*
C20	0.5454 (4)	0.3065 (4)	0.55163 (18)	0.0598 (9)
H20	0.5000	0.3873	0.5500	0.072*
C21	0.5387 (5)	0.2287 (4)	0.50119 (17)	0.0668 (11)
H21	0.4888	0.2555	0.4649	0.080*
C22	0.6049 (5)	0.1122 (4)	0.50404 (16)	0.0688 (11)
H22	0.6016	0.0585	0.4694	0.083*
C23	0.6765 (4)	0.0727 (3)	0.55703 (15)	0.0529 (8)
H23	0.7205	−0.0086	0.5586	0.063*
C24	0.8137 (3)	0.3888 (2)	0.84308 (12)	0.0316 (5)
C25	0.7587 (4)	0.5348 (3)	0.92114 (14)	0.0446 (7)
H25A	0.7974	0.6061	0.8975	0.067*
H25B	0.8397	0.5016	0.9473	0.067*
H25C	0.6736	0.5623	0.9467	0.067*
C26	0.5022 (3)	0.0412 (3)	0.73991 (14)	0.0387 (6)
H26A	0.4606	0.0560	0.6989	0.058*
H26B	0.4192	0.0394	0.7698	0.058*
H26C	0.5558	−0.0393	0.7405	0.058*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0366 (12)	0.0751 (16)	0.0676 (15)	−0.0174 (11)	0.0058 (11)	−0.0342 (14)
O2	0.0370 (11)	0.0398 (11)	0.0411 (10)	−0.0007 (8)	0.0007 (8)	−0.0131 (9)
N1	0.0321 (11)	0.0329 (11)	0.0294 (11)	−0.0004 (9)	−0.0020 (8)	−0.0042 (9)
C1	0.0296 (12)	0.0307 (13)	0.0324 (13)	−0.0007 (10)	−0.0031 (10)	−0.0002 (10)
C2	0.0284 (12)	0.0276 (12)	0.0299 (12)	0.0008 (10)	−0.0038 (10)	0.0016 (10)
C3	0.0283 (12)	0.0273 (12)	0.0308 (12)	0.0015 (10)	−0.0030 (10)	−0.0002 (10)
C4	0.0301 (13)	0.0303 (13)	0.0325 (13)	0.0006 (10)	−0.0016 (10)	−0.0015 (10)
C5	0.0318 (13)	0.0263 (12)	0.0339 (13)	−0.0025 (10)	0.0008 (10)	−0.0031 (10)

C6	0.0329 (14)	0.0388 (15)	0.0382 (15)	−0.0016 (11)	−0.0021 (11)	0.0008 (12)
C7	0.0303 (14)	0.0480 (18)	0.0569 (19)	−0.0003 (13)	0.0058 (13)	−0.0027 (14)
C8	0.0483 (17)	0.0467 (17)	0.0452 (17)	−0.0068 (13)	0.0180 (14)	−0.0043 (14)
C9	0.0546 (19)	0.0511 (18)	0.0317 (14)	−0.0035 (15)	0.0047 (13)	0.0018 (13)
C10	0.0349 (14)	0.0403 (15)	0.0354 (14)	−0.0021 (12)	−0.0004 (11)	0.0008 (11)
C11	0.0321 (13)	0.0350 (14)	0.0285 (12)	−0.0026 (10)	0.0000 (10)	−0.0051 (10)
C12	0.0409 (15)	0.0354 (15)	0.0443 (15)	−0.0004 (12)	0.0041 (12)	−0.0057 (13)
C13	0.0517 (18)	0.0359 (16)	0.0436 (16)	−0.0072 (12)	0.0050 (14)	0.0007 (12)
C14	0.0412 (16)	0.0508 (17)	0.0320 (13)	−0.0128 (12)	0.0068 (11)	−0.0053 (13)
C15	0.0316 (15)	0.0529 (17)	0.0413 (15)	0.0013 (12)	0.0022 (11)	−0.0034 (13)
C16	0.0351 (14)	0.0402 (15)	0.0406 (15)	0.0010 (11)	−0.0015 (11)	0.0052 (12)
C17	0.0365 (14)	0.0373 (14)	0.0328 (13)	0.0038 (11)	−0.0005 (11)	−0.0079 (11)
C18	0.0338 (14)	0.0413 (15)	0.0319 (14)	−0.0047 (12)	0.0047 (10)	0.0002 (11)
C19	0.0449 (16)	0.0459 (18)	0.0443 (16)	−0.0021 (14)	0.0027 (13)	0.0018 (13)
C20	0.058 (2)	0.062 (2)	0.060 (2)	−0.0049 (17)	−0.0040 (17)	0.0243 (18)
C21	0.069 (2)	0.094 (3)	0.0374 (17)	−0.016 (2)	−0.0051 (16)	0.0245 (19)
C22	0.086 (3)	0.090 (3)	0.0295 (16)	−0.013 (2)	−0.0009 (17)	−0.0045 (17)
C23	0.064 (2)	0.058 (2)	0.0362 (15)	0.0005 (16)	0.0042 (14)	−0.0082 (15)
C24	0.0309 (13)	0.0313 (13)	0.0325 (13)	−0.0025 (10)	−0.0015 (10)	0.0001 (11)
C25	0.0581 (19)	0.0387 (16)	0.0369 (15)	0.0006 (14)	−0.0044 (14)	−0.0110 (12)
C26	0.0351 (14)	0.0369 (14)	0.0440 (16)	−0.0066 (11)	−0.0027 (12)	−0.0084 (12)

Geometric parameters (Å, º)

O1—C24	1.202 (3)	C13—H13	0.9500
O2—C24	1.337 (3)	C13—C14	1.376 (4)
O2—C25	1.442 (3)	C14—H14	0.9500
N1—C1	1.379 (3)	C14—C15	1.378 (4)
N1—C4	1.368 (3)	C15—H15	0.9500
N1—C17	1.465 (3)	C15—C16	1.390 (4)
C1—C2	1.377 (4)	C16—H16	0.9500
C1—C26	1.499 (4)	C17—H17A	0.9900
C2—C3	1.433 (3)	C17—H17B	0.9900
C2—C5	1.477 (4)	C17—C18	1.511 (4)
C3—C4	1.388 (4)	C18—C19	1.381 (4)
C3—C24	1.465 (4)	C18—C23	1.381 (4)
C4—C11	1.482 (4)	C19—H19	0.9500
C5—C6	1.394 (4)	C19—C20	1.392 (5)
C5—C10	1.395 (4)	C20—H20	0.9500
C6—H6	0.9500	C20—C21	1.380 (6)
C6—C7	1.387 (4)	C21—H21	0.9500
C7—H7	0.9500	C21—C22	1.374 (6)
C7—C8	1.381 (5)	C22—H22	0.9500
C8—H8	0.9500	C22—C23	1.383 (5)
C8—C9	1.385 (5)	C23—H23	0.9500
C9—H9	0.9500	C25—H25A	0.9800
C9—C10	1.385 (4)	C25—H25B	0.9800
C10—H10	0.9500	C25—H25C	0.9800
C11—C12	1.394 (4)	C26—H26A	0.9800
C11—C16	1.386 (4)	C26—H26B	0.9800

C12—H12	0.9500	C26—H26C	0.9800
C12—C13	1.381 (4)		

C24—O2—C25	116.0 (2)	C14—C15—H15	119.9
C1—N1—C17	124.5 (2)	C14—C15—C16	120.2 (3)
C4—N1—C1	109.9 (2)	C16—C15—H15	119.9
C4—N1—C17	125.6 (2)	C11—C16—C15	120.4 (3)
N1—C1—C26	121.2 (2)	C11—C16—H16	119.8
C2—C1—N1	108.3 (2)	C15—C16—H16	119.8
C2—C1—C26	130.3 (3)	N1—C17—H17A	108.6
C1—C2—C3	106.6 (2)	N1—C17—H17B	108.6
C1—C2—C5	124.3 (2)	N1—C17—C18	114.8 (2)
C3—C2—C5	128.8 (2)	H17A—C17—H17B	107.5
C2—C3—C24	129.3 (2)	C18—C17—H17A	108.6
C4—C3—C2	107.7 (2)	C18—C17—H17B	108.6
C4—C3—C24	123.0 (2)	C19—C18—C17	123.0 (3)
N1—C4—C3	107.4 (2)	C23—C18—C17	118.1 (3)
N1—C4—C11	122.5 (2)	C23—C18—C19	118.9 (3)
C3—C4—C11	129.8 (2)	C18—C19—H19	119.9
C6—C5—C2	120.8 (2)	C18—C19—C20	120.3 (3)
C6—C5—C10	118.2 (2)	C20—C19—H19	119.9
C10—C5—C2	120.9 (2)	C19—C20—H20	119.8
C5—C6—H6	119.6	C21—C20—C19	120.3 (4)
C7—C6—C5	120.9 (3)	C21—C20—H20	119.8
C7—C6—H6	119.6	C20—C21—H21	120.4
C6—C7—H7	119.8	C22—C21—C20	119.3 (3)
C8—C7—C6	120.3 (3)	C22—C21—H21	120.4
C8—C7—H7	119.8	C21—C22—H22	119.8
C7—C8—H8	120.3	C21—C22—C23	120.5 (4)
C7—C8—C9	119.4 (3)	C23—C22—H22	119.8
C9—C8—H8	120.3	C18—C23—C22	120.7 (4)
C8—C9—H9	119.7	C18—C23—H23	119.6
C10—C9—C8	120.5 (3)	C22—C23—H23	119.6
C10—C9—H9	119.7	O1—C24—O2	122.4 (3)
C5—C10—H10	119.7	O1—C24—C3	125.0 (3)
C9—C10—C5	120.6 (3)	O2—C24—C3	112.6 (2)
C9—C10—H10	119.7	O2—C25—H25A	109.5
C12—C11—C4	119.8 (2)	O2—C25—H25B	109.5
C16—C11—C4	121.5 (2)	O2—C25—H25C	109.5
C16—C11—C12	118.7 (3)	H25A—C25—H25B	109.5
C11—C12—H12	119.7	H25A—C25—H25C	109.5
C13—C12—C11	120.5 (3)	H25B—C25—H25C	109.5
C13—C12—H12	119.7	C1—C26—H26A	109.5
C12—C13—H13	119.8	C1—C26—H26B	109.5
C14—C13—C12	120.4 (3)	C1—C26—H26C	109.5
C14—C13—H13	119.8	H26A—C26—H26B	109.5
C13—C14—H14	120.1	H26A—C26—H26C	109.5
C13—C14—C15	119.8 (3)	H26B—C26—H26C	109.5
C15—C14—H14	120.1		

N1—C1—C2—C3	−0.3 (3)	C5—C2—C3—C24	−4.4 (4)
N1—C1—C2—C5	−175.1 (2)	C5—C6—C7—C8	−0.2 (5)
N1—C4—C11—C12	105.7 (3)	C6—C5—C10—C9	0.5 (4)
N1—C4—C11—C16	−74.9 (4)	C6—C7—C8—C9	1.1 (5)
N1—C17—C18—C19	21.3 (4)	C7—C8—C9—C10	−1.2 (5)
N1—C17—C18—C23	−161.1 (3)	C8—C9—C10—C5	0.4 (5)
C1—N1—C4—C3	0.5 (3)	C10—C5—C6—C7	−0.6 (4)
C1—N1—C4—C11	−174.4 (2)	C11—C12—C13—C14	0.9 (5)
C1—N1—C17—C18	80.0 (3)	C12—C11—C16—C15	0.1 (4)
C1—C2—C3—C4	0.6 (3)	C12—C13—C14—C15	0.0 (5)
C1—C2—C3—C24	−179.0 (3)	C13—C14—C15—C16	−0.9 (4)
C1—C2—C5—C6	−59.7 (4)	C14—C15—C16—C11	0.8 (5)
C1—C2—C5—C10	118.3 (3)	C16—C11—C12—C13	−1.0 (4)
C2—C3—C4—N1	−0.7 (3)	C17—N1—C1—C2	178.6 (2)
C2—C3—C4—C11	173.8 (3)	C17—N1—C1—C26	3.4 (4)
C2—C3—C24—O1	157.7 (3)	C17—N1—C4—C3	−178.2 (2)
C2—C3—C24—O2	−22.4 (4)	C17—N1—C4—C11	6.9 (4)
C2—C5—C6—C7	177.4 (3)	C17—C18—C19—C20	177.1 (3)
C2—C5—C10—C9	−177.5 (3)	C17—C18—C23—C22	−176.7 (3)
C3—C2—C5—C6	126.6 (3)	C18—C19—C20—C21	0.0 (5)
C3—C2—C5—C10	−55.4 (4)	C19—C18—C23—C22	0.9 (5)
C3—C4—C11—C12	−67.9 (4)	C19—C20—C21—C22	−0.1 (6)
C3—C4—C11—C16	111.5 (3)	C20—C21—C22—C23	0.6 (6)
C4—N1—C1—C2	−0.1 (3)	C21—C22—C23—C18	−1.0 (6)
C4—N1—C1—C26	−175.3 (2)	C23—C18—C19—C20	−0.4 (5)
C4—N1—C17—C18	−101.5 (3)	C24—C3—C4—N1	178.9 (2)
C4—C3—C24—O1	−21.8 (4)	C24—C3—C4—C11	−6.7 (4)
C4—C3—C24—O2	158.1 (2)	C25—O2—C24—O1	1.6 (4)
C4—C11—C12—C13	178.4 (3)	C25—O2—C24—C3	−178.3 (2)
C4—C11—C16—C15	−179.3 (3)	C26—C1—C2—C3	174.3 (3)
C5—C2—C3—C4	175.1 (2)	C26—C1—C2—C5	−0.6 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C17—H17*B*···O1^{i}	0.99	2.56	3.177 (3)	120
C26—H26*A*···O2^{ii}	0.98	2.59	3.383 (3)	138

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