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Methyl 1-methyl-3-phenyl-1,2,3,3a,4,9b-hexahydrobenzo[*f*]chromeno[4,3-*b*]-pyrrole-3a-carboxylate

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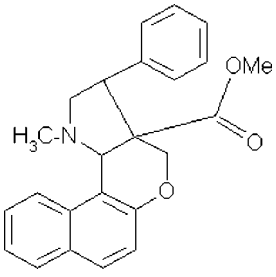
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.040; wR factor = 0.107; data-to-parameter ratio = 13.7.

In the title compound, $C_{24}H_{23}NO_3$, the dihedral angle between the naphthalene ring system and the phenyl ring is 76.82 (6)°. The pyrrolidine ring adopts an envelope conformation. In the crystal, weak intermolecular C—H···O and C—H···π interactions are observed.

Related literature

For the biological activity of chromenopyrrole, see: Caine (1993); Tidey (1992); Carlson (1993); Sokoloff *et al.* (1990); Wilner (1985); Sobral & Rocha Gonsalves (2001*a*,*b*); Brockmann & Tour (1995); Suslick *et al.* (1992); Di Natale *et al.* (1998). For a related structure, see: Nirmala *et al.* (2008). For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{24}H_{23}NO_3$
M_r = 373.43
Monoclinic, $P2_1/n$
a = 13.2332 (6) Å
b = 10.3574 (4) Å
c = 15.0865 (6) Å
β = 111.530 (2)°
V = 1923.50 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 K
0.25 × 0.20 × 0.15 mm

Data collection

Bruker Kappa APEX2 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.979, T_{max} = 0.987
19089 measured reflections
3499 independent reflections
2413 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.107
S = 1.02
3499 reflections
255 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15···O2^{i}	0.98	2.53	3.347 (2)	141
C16—H16C···Cg^{ii}	0.96	2.79	3.689 (4)	156

Symmetry codes: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+1, -y+1, -z+1$. Cg is the centroid of the C4–C9 ring.

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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2404).

References

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Brockmann, T. W. & Tour, J. M. (1995). *J. Am. Chem. Soc.* **117**, 4437–4447.
Bruker (2004). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
Caine, B. (1993). *Science*, **260**, 1814–1816.
Carlson, J. (1993). *Neur. Transm.* **94**, 11–19.
Di Natale, C., Paolesse, R., Macagnano, A., Mantini, A., Goletti, C., Tarizzo, E. & Amico, A. (1998). *Sens. Actuators*, B**50**, 162–168.
Nirmala, S., Kamala, E. T. S., Sudha, L., Ramesh, E. & Raghunathan, R. (2008). *Acta Cryst.* E**64**, o649.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sobral, A. J. F. N. & Rocha Gonsalves, A. M. D. A. (2001*a*). *J. Porphyrins Phthalocyanines*, **5**, 428–430.
Sobral, A. J. F. N. & Rocha Gonsalves, A. M. D. A. (2001*b*). *J. Porphyrins Phthalocyanines*, **5**, 861–866.
Sokoloff, P., Giros, B., Martres, M. P., Bouthenet, M. L. & Schwartz, J. C. (1990). *Nature (London)*, **347**, 147–151.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Suslick, K. S., Chen, C. T., Meredith, G. R. & Cheng, L. T. (1992). *J. Am. Chem. Soc.* **114**, 6928–6930.
Tidey, J. W. (1992). *Behav. Pharm.* **3**, 553–566.
Wilner, P. (1985). *Clin. Neuropharm.* **18**, Suppl. 1, 549–556.

supporting information

Acta Cryst. (2009). E**65**, o1033 [doi:10.1107/S1600536809012914]

Methyl 1-methyl-3-phenyl-1,2,3,3a,4,9b-hexahydrobenzo[*f*]chromeno[4,3-*b*]pyrrole-3a-carboxylate

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S1. Comment

Chromenopyrrole compounds are used in the treatment of impulsive disorders (Caine, 1993), aggressiveness (Tidey, 1992), parkinson's disease (Carlson, 1993), psychoses, memory disorders (Sokoloff *et al.*, 1990), anxiety and depression (Wilner, 1985). Pyrroles are also very useful precursors in porphyrin synthesis (Sobral & Rocha Gonsalves, 2001*a*,*b*), and as monomers for polymer chemistry (Brockmann & Tour, 1995), with applications ranging from nonlinear optical materials (Suslick *et al.*, 1992) to electronic noses (Di Natale *et al.*, 1998).

The geometric parameters of the title molecule (Fig. 1) agree well with reported similar structure (Nirmala *et al.*, 2008). The six-membered heterocyclic ring [C7/O1/C11/C12/C13/C8] of the benzochromenopyrrole moiety adopts a half-chair conformation [O1—C7—C8—C13 = 0.5 (2)° and O1—C11—C12—C13 = -60.09 (17)°]. The sum of bond angles around N1 [332.37 (14)°] indicates the sp^3 hybridized state of atom N1 in the molecule. The C16—N1—C13—C12 torsion angle is -173.40 (14)°, which corresponds to an antiperiplanar conformation.

The crystal packing is stabilized by weak intramolecular C—H···O and C—H···N interactions. In addition, the structure is stabilized by weak intermolecular C—H···O and C—H···π (C16—H16C···*Cg*; *Cg* is the centroid of ring defined by the atoms C4–C9) interactions (Table 1). The C11—H11A···N1 and C13—H13···O3 interactions each generate an S(5) graph set motif (Bernstein *et al.*, 1995).

S2. Experimental

A mixture of (*z*)-methyl-5-(1-formylnathalen-2-yl-)-3-phenylpent -2-enoate and sarcosine 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.

S3. Refinement

H atoms were positioned geometrically and refined using riding model, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic C—H, C—H = 0.98 Å and U_{iso}(H) = 1.2U_{eq}(C) for C—H, C—H = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for CH_2, and C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for CH_3.

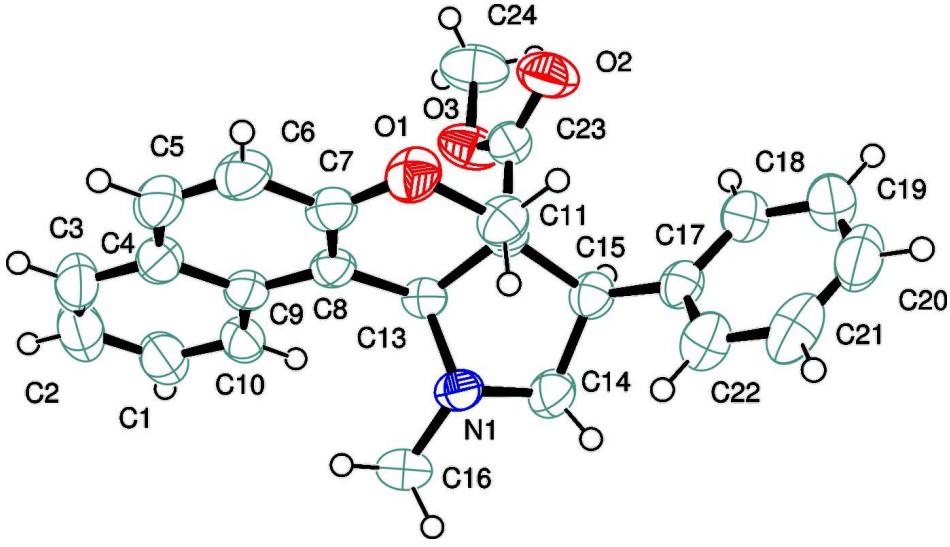

Figure 1

The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms.

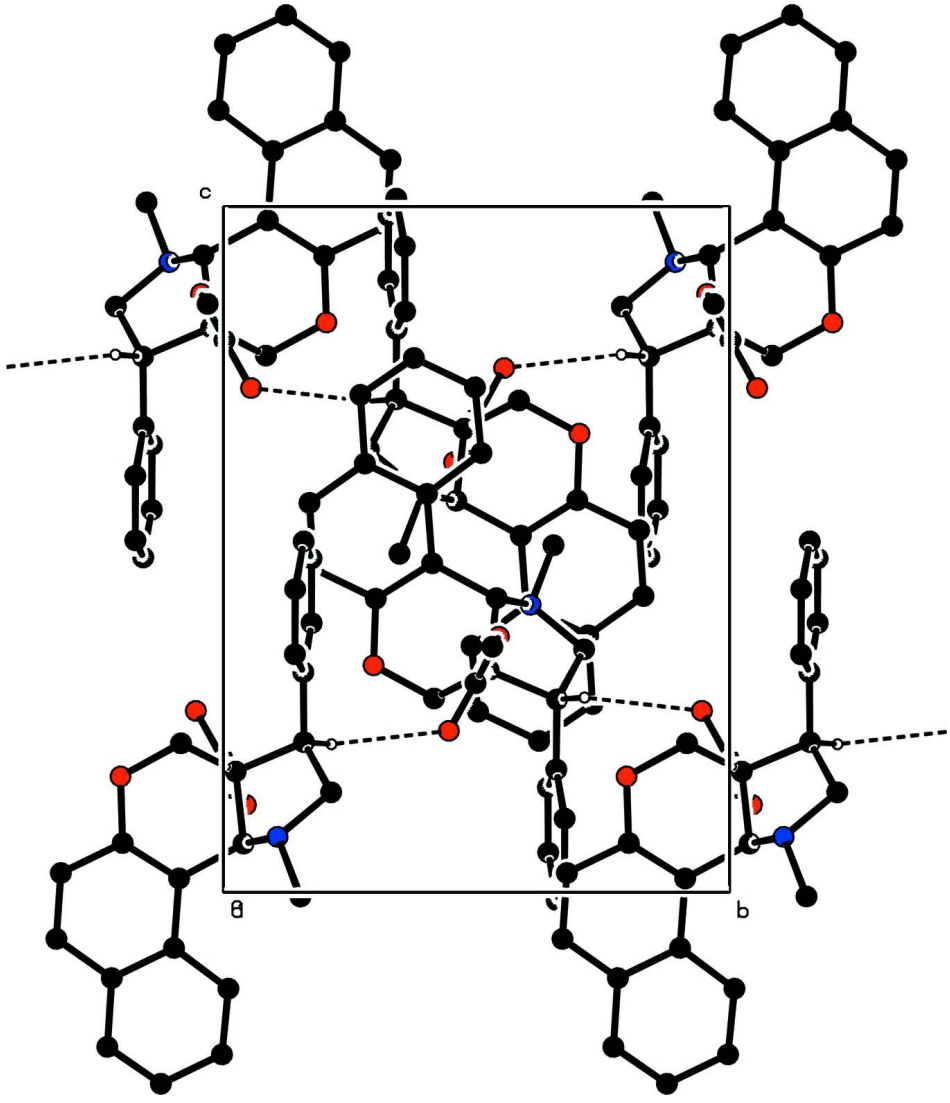

Figure 2

The packing of (I), viewed down the *a* axis. Hydrogen bonds are shown as dashed lines.

Methyl 1-methyl-3-phenyl-1,2,3,3a,4,9b- hexahydrobenzo[*f*]chromeno[4,3-*b*]pyrrole-3a-carboxylate

Crystal data

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b = 10.3574 (4) Å
c = 15.0865 (6) Å
β = 111.530 (2)°
V = 1923.50 (14) Å^3
Z = 4
$F(000)$ = 792
D_x = 1.290 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3865 reflections
θ = 1.8–25.3°
μ = 0.09 mm^{-1}
T = 293 K
Block, colourless
0.25 × 0.20 × 0.15 mm

Data collection

Bruker Kappa APEX2 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} = 0.979, T_{max} = 0.987

19089 measured reflections
3499 independent reflections
2413 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 25.3°, θ_{min} = 2.4°
h = −15→15
k = −11→12
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.107
S = 1.02
3499 reflections
255 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
$w = 1/[\sigma^2(F_o^2) + (0.0458P)^2 + 0.3587P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 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}
O1	0.87620 (10)	0.79656 (11)	0.16896 (8)	0.0560 (3)
O3	0.64358 (10)	1.04425 (13)	0.12731 (9)	0.0610 (4)
C8	0.80155 (13)	0.91239 (15)	0.02018 (11)	0.0404 (4)
O2	0.72839 (11)	0.94550 (14)	0.26458 (9)	0.0684 (4)
C7	0.83173 (14)	0.80090 (16)	0.07191 (12)	0.0473 (4)
N1	0.91939 (11)	1.10692 (13)	0.08087 (9)	0.0452 (4)
C13	0.81799 (13)	1.03987 (15)	0.07102 (10)	0.0388 (4)
H13	0.7558	1.0965	0.0393	0.047*
C9	0.74815 (13)	0.90220 (16)	−0.08105 (12)	0.0452 (4)
C11	0.91380 (14)	0.91616 (15)	0.21733 (12)	0.0483 (4)
H11A	0.9827	0.9387	0.2124	0.058*
H11B	0.9258	0.9059	0.2843	0.058*
C10	0.70597 (14)	1.00976 (19)	−0.14052 (12)	0.0508 (4)
H10	0.7133	1.0915	−0.1134	0.061*
C4	0.73409 (15)	0.77937 (18)	−0.12524 (13)	0.0553 (5)
C12	0.83340 (13)	1.02418 (15)	0.17618 (10)	0.0394 (4)

C23	0.73092 (14)	0.99806 (16)	0.19506 (11)	0.0439 (4)
C6	0.81600 (17)	0.67864 (17)	0.02815 (15)	0.0605 (5)
H6	0.8373	0.6044	0.0650	0.073*
C17	0.95781 (14)	1.15779 (15)	0.32102 (11)	0.0440 (4)
C15	0.88052 (14)	1.15911 (15)	0.21892 (11)	0.0448 (4)
H15	0.8187	1.2134	0.2160	0.054*
C5	0.76969 (17)	0.66982 (19)	−0.06782 (15)	0.0665 (6)
H5	0.7613	0.5889	−0.0964	0.080*
C16	0.93000 (15)	1.15213 (18)	−0.00619 (12)	0.0555 (5)
H16A	0.8733	1.2130	−0.0371	0.083*
H16B	0.9244	1.0802	−0.0479	0.083*
H16C	0.9993	1.1931	0.0087	0.083*
C3	0.68054 (18)	0.7705 (2)	−0.22541 (15)	0.0715 (6)
H3	0.6717	0.6900	−0.2546	0.086*
C22	1.06811 (15)	1.14119 (17)	0.34720 (13)	0.0580 (5)
H22	1.0977	1.1295	0.3006	0.070*
C1	0.65478 (16)	0.9971 (2)	−0.23651 (13)	0.0629 (5)
H1	0.6280	1.0699	−0.2738	0.076*
C2	0.64222 (18)	0.8763 (3)	−0.27927 (15)	0.0753 (6)
H2	0.6075	0.8685	−0.3449	0.090*
C14	0.92485 (17)	1.21276 (17)	0.14582 (12)	0.0580 (5)
H14A	0.8811	1.2850	0.1117	0.070*
H14B	0.9992	1.2417	0.1771	0.070*
C18	0.91714 (17)	1.17418 (17)	0.39259 (12)	0.0571 (5)
H18	0.8428	1.1855	0.3765	0.069*
C19	0.9842 (2)	1.1741 (2)	0.48683 (14)	0.0760 (7)
H19	0.9550	1.1846	0.5338	0.091*
C21	1.13528 (18)	1.14174 (19)	0.44215 (15)	0.0725 (6)
H21	1.2097	1.1306	0.4588	0.087*
C20	1.0936 (2)	1.1585 (2)	0.51178 (15)	0.0784 (7)
H20	1.1392	1.1594	0.5756	0.094*
C24	0.54215 (16)	1.0313 (2)	0.14187 (16)	0.0749 (6)
H24A	0.5298	0.9421	0.1518	0.112*
H24B	0.4839	1.0628	0.0868	0.112*
H24C	0.5453	1.0806	0.1967	0.112*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0678 (9)	0.0358 (7)	0.0620 (8)	0.0033 (6)	0.0211 (6)	0.0046 (6)
O3	0.0449 (7)	0.0785 (9)	0.0673 (8)	0.0114 (7)	0.0296 (6)	0.0219 (7)
C8	0.0387 (9)	0.0373 (9)	0.0525 (10)	−0.0033 (7)	0.0254 (8)	−0.0041 (8)
O2	0.0685 (9)	0.0824 (10)	0.0587 (8)	−0.0099 (7)	0.0284 (7)	0.0197 (7)
C7	0.0473 (11)	0.0413 (10)	0.0600 (11)	−0.0024 (8)	0.0278 (9)	−0.0016 (8)
N1	0.0440 (9)	0.0439 (8)	0.0500 (8)	−0.0079 (6)	0.0199 (6)	0.0019 (6)
C13	0.0379 (9)	0.0367 (9)	0.0441 (9)	0.0004 (7)	0.0180 (7)	0.0023 (7)
C9	0.0407 (10)	0.0490 (10)	0.0540 (10)	−0.0075 (8)	0.0270 (8)	−0.0092 (8)
C11	0.0501 (11)	0.0396 (10)	0.0527 (10)	0.0019 (8)	0.0159 (8)	0.0033 (8)

C10	0.0472 (10)	0.0607 (12)	0.0481 (10)	−0.0038 (9)	0.0217 (8)	−0.0073 (9)
C4	0.0563 (12)	0.0537 (12)	0.0659 (12)	−0.0100 (9)	0.0343 (10)	−0.0151 (10)
C12	0.0400 (9)	0.0372 (9)	0.0411 (8)	0.0006 (7)	0.0151 (7)	0.0032 (7)
C23	0.0505 (11)	0.0385 (9)	0.0441 (9)	−0.0032 (8)	0.0190 (8)	−0.0006 (8)
C6	0.0731 (14)	0.0364 (10)	0.0847 (14)	−0.0042 (9)	0.0437 (11)	−0.0044 (9)
C17	0.0488 (11)	0.0331 (9)	0.0479 (9)	−0.0020 (8)	0.0150 (8)	−0.0029 (7)
C15	0.0481 (10)	0.0374 (9)	0.0470 (9)	0.0000 (8)	0.0151 (8)	−0.0005 (7)
C5	0.0817 (15)	0.0477 (12)	0.0858 (15)	−0.0156 (11)	0.0492 (12)	−0.0239 (11)
C16	0.0533 (12)	0.0587 (12)	0.0626 (11)	−0.0069 (9)	0.0310 (9)	0.0072 (9)
C3	0.0717 (15)	0.0794 (16)	0.0716 (14)	−0.0169 (12)	0.0357 (12)	−0.0354 (12)
C22	0.0532 (12)	0.0536 (12)	0.0621 (12)	−0.0017 (9)	0.0151 (9)	−0.0105 (9)
C1	0.0578 (12)	0.0812 (15)	0.0518 (11)	0.0006 (10)	0.0225 (9)	−0.0056 (10)
C2	0.0688 (15)	0.1018 (19)	0.0555 (12)	−0.0036 (13)	0.0228 (11)	−0.0226 (13)
C14	0.0734 (14)	0.0471 (11)	0.0495 (10)	−0.0171 (9)	0.0178 (9)	−0.0005 (8)
C18	0.0661 (13)	0.0527 (11)	0.0553 (11)	−0.0083 (9)	0.0255 (10)	−0.0086 (9)
C19	0.104 (2)	0.0731 (15)	0.0519 (12)	−0.0254 (13)	0.0300 (13)	−0.0113 (10)
C21	0.0602 (14)	0.0545 (13)	0.0789 (15)	−0.0040 (10)	−0.0026 (12)	−0.0073 (11)
C20	0.103 (2)	0.0590 (14)	0.0502 (12)	−0.0214 (13)	0.0010 (13)	−0.0019 (10)
C24	0.0524 (13)	0.0869 (16)	0.1010 (16)	0.0095 (11)	0.0467 (12)	0.0171 (13)

Geometric parameters (Å, º)

O1—C7	1.3637 (19)	C17—C18	1.382 (2)
O1—C11	1.4311 (19)	C17—C15	1.504 (2)
O3—C23	1.320 (2)	C15—C14	1.531 (2)
O3—C24	1.444 (2)	C15—H15	0.9800
C8—C7	1.369 (2)	C5—H5	0.9300
C8—C9	1.432 (2)	C16—H16A	0.9600
C8—C13	1.502 (2)	C16—H16B	0.9600
O2—C23	1.1931 (18)	C16—H16C	0.9600
C7—C6	1.408 (2)	C3—C2	1.347 (3)
N1—C16	1.449 (2)	C3—H3	0.9300
N1—C14	1.454 (2)	C22—C21	1.381 (3)
N1—C13	1.469 (2)	C22—H22	0.9300
C13—C12	1.532 (2)	C1—C2	1.389 (3)
C13—H13	0.9800	C1—H1	0.9300
C9—C10	1.411 (2)	C2—H2	0.9300
C9—C4	1.417 (2)	C14—H14A	0.9700
C11—C12	1.511 (2)	C14—H14B	0.9700
C11—H11A	0.9700	C18—C19	1.372 (3)
C11—H11B	0.9700	C18—H18	0.9300
C10—C1	1.361 (2)	C19—C20	1.364 (3)
C10—H10	0.9300	C19—H19	0.9300
C4—C5	1.400 (3)	C21—C20	1.365 (3)
C4—C3	1.417 (3)	C21—H21	0.9300
C12—C23	1.509 (2)	C20—H20	0.9300
C12—C15	1.569 (2)	C24—H24A	0.9600
C6—C5	1.352 (3)	C24—H24B	0.9600

C6—H6	0.9300	C24—H24C	0.9600
C17—C22	1.376 (2)		
C7—O1—C11	116.82 (12)	C14—C15—C12	103.10 (12)
C23—O3—C24	116.58 (14)	C17—C15—H15	107.1
C7—C8—C9	118.20 (15)	C14—C15—H15	107.1
C7—C8—C13	119.55 (14)	C12—C15—H15	107.1
C9—C8—C13	122.11 (14)	C6—C5—C4	121.67 (17)
O1—C7—C8	124.11 (15)	C6—C5—H5	119.2
O1—C7—C6	113.89 (16)	C4—C5—H5	119.2
C8—C7—C6	121.97 (16)	N1—C16—H16A	109.5
C16—N1—C14	111.70 (13)	N1—C16—H16B	109.5
C16—N1—C13	116.73 (13)	H16A—C16—H16B	109.5
C14—N1—C13	104.01 (13)	N1—C16—H16C	109.5
N1—C13—C8	115.02 (13)	H16A—C16—H16C	109.5
N1—C13—C12	100.13 (12)	H16B—C16—H16C	109.5
C8—C13—C12	112.01 (13)	C2—C3—C4	121.4 (2)
N1—C13—H13	109.8	C2—C3—H3	119.3
C8—C13—H13	109.8	C4—C3—H3	119.3
C12—C13—H13	109.8	C17—C22—C21	120.56 (19)
C10—C9—C4	117.20 (15)	C17—C22—H22	119.7
C10—C9—C8	123.04 (15)	C21—C22—H22	119.7
C4—C9—C8	119.75 (16)	C10—C1—C2	120.6 (2)
O1—C11—C12	111.76 (13)	C10—C1—H1	119.7
O1—C11—H11A	109.3	C2—C1—H1	119.7
C12—C11—H11A	109.3	C3—C2—C1	119.85 (19)
O1—C11—H11B	109.3	C3—C2—H2	120.1
C12—C11—H11B	109.3	C1—C2—H2	120.1
H11A—C11—H11B	107.9	N1—C14—C15	105.93 (13)
C1—C10—C9	121.78 (18)	N1—C14—H14A	110.6
C1—C10—H10	119.1	C15—C14—H14A	110.6
C9—C10—H10	119.1	N1—C14—H14B	110.6
C5—C4—C9	118.71 (17)	C15—C14—H14B	110.6
C5—C4—C3	122.04 (19)	H14A—C14—H14B	108.7
C9—C4—C3	119.19 (19)	C19—C18—C17	121.3 (2)
C23—C12—C11	109.62 (13)	C19—C18—H18	119.3
C23—C12—C13	115.29 (13)	C17—C18—H18	119.3
C11—C12—C13	108.05 (13)	C20—C19—C18	120.2 (2)
C23—C12—C15	109.34 (13)	C20—C19—H19	119.9
C11—C12—C15	112.14 (13)	C18—C19—H19	119.9
C13—C12—C15	102.29 (12)	C20—C21—C22	120.7 (2)
O2—C23—O3	123.16 (16)	C20—C21—H21	119.7
O2—C23—C12	124.39 (16)	C22—C21—H21	119.7
O3—C23—C12	112.40 (13)	C19—C20—C21	119.35 (19)
C5—C6—C7	119.59 (18)	C19—C20—H20	120.3
C5—C6—H6	120.2	C21—C20—H20	120.3
C7—C6—H6	120.2	O3—C24—H24A	109.5
C22—C17—C18	117.86 (16)	O3—C24—H24B	109.5

C22—C17—C15	123.11 (16)	H24A—C24—H24B	109.5
C18—C17—C15	119.03 (16)	O3—C24—H24C	109.5
C17—C15—C14	116.40 (15)	H24A—C24—H24C	109.5
C17—C15—C12	115.53 (13)	H24B—C24—H24C	109.5
C11—O1—C7—C8	−13.5 (2)	C13—C12—C23—O2	155.96 (16)
C11—O1—C7—C6	168.25 (15)	C15—C12—C23—O2	−89.50 (19)
C9—C8—C7—O1	−175.27 (14)	C11—C12—C23—O3	−148.53 (14)
C13—C8—C7—O1	0.5 (2)	C13—C12—C23—O3	−26.37 (19)
C9—C8—C7—C6	2.8 (2)	C15—C12—C23—O3	88.17 (16)
C13—C8—C7—C6	178.56 (16)	O1—C7—C6—C5	178.20 (16)
C16—N1—C13—C8	66.33 (19)	C8—C7—C6—C5	−0.1 (3)
C14—N1—C13—C8	−170.14 (13)	C22—C17—C15—C14	−31.9 (2)
C16—N1—C13—C12	−173.44 (13)	C18—C17—C15—C14	148.01 (16)
C14—N1—C13—C12	−49.91 (15)	C22—C17—C15—C12	89.3 (2)
C7—C8—C13—N1	94.95 (17)	C18—C17—C15—C12	−90.82 (19)
C9—C8—C13—N1	−89.46 (18)	C23—C12—C15—C17	88.85 (17)
C7—C8—C13—C12	−18.5 (2)	C11—C12—C15—C17	−32.95 (19)
C9—C8—C13—C12	157.09 (14)	C13—C12—C15—C17	−148.48 (14)
C7—C8—C9—C10	174.89 (15)	C23—C12—C15—C14	−143.05 (14)
C13—C8—C9—C10	−0.8 (2)	C11—C12—C15—C14	95.15 (16)
C7—C8—C9—C4	−3.9 (2)	C13—C12—C15—C14	−20.38 (16)
C13—C8—C9—C4	−179.52 (14)	C7—C6—C5—C4	−1.7 (3)
C7—O1—C11—C12	44.22 (19)	C9—C4—C5—C6	0.5 (3)
C4—C9—C10—C1	−0.7 (2)	C3—C4—C5—C6	−176.74 (18)
C8—C9—C10—C1	−179.46 (15)	C5—C4—C3—C2	176.87 (19)
C10—C9—C4—C5	−176.58 (16)	C9—C4—C3—C2	−0.4 (3)
C8—C9—C4—C5	2.3 (2)	C18—C17—C22—C21	−0.3 (3)
C10—C9—C4—C3	0.8 (2)	C15—C17—C22—C21	179.54 (17)
C8—C9—C4—C3	179.63 (15)	C9—C10—C1—C2	0.1 (3)
O1—C11—C12—C23	66.29 (17)	C4—C3—C2—C1	−0.1 (3)
O1—C11—C12—C13	−60.09 (17)	C10—C1—C2—C3	0.3 (3)
O1—C11—C12—C15	−172.07 (13)	C16—N1—C14—C15	164.03 (14)
N1—C13—C12—C23	160.94 (13)	C13—N1—C14—C15	37.29 (17)
C8—C13—C12—C23	−76.68 (17)	C17—C15—C14—N1	118.28 (16)
N1—C13—C12—C11	−76.07 (15)	C12—C15—C14—N1	−9.28 (17)
C8—C13—C12—C11	46.31 (17)	C22—C17—C18—C19	0.0 (3)
N1—C13—C12—C15	42.39 (15)	C15—C17—C18—C19	−179.84 (17)
C8—C13—C12—C15	164.78 (13)	C17—C18—C19—C20	0.5 (3)
C24—O3—C23—O2	1.5 (3)	C17—C22—C21—C20	0.1 (3)
C24—O3—C23—C12	−176.18 (15)	C18—C19—C20—C21	−0.7 (3)
C11—C12—C23—O2	33.8 (2)	C22—C21—C20—C19	0.4 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11*A*···N1	0.97	2.54	2.874 (2)	100
C13—H13···O3	0.98	2.39	2.7366 (19)	100

C15—H15···O2^{i}	0.98	2.53	3.347 (2)	141
C16—H16*C*···*Cg*^{ii}	0.96	2.79	3.689 (4)	156

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