IUCrData

ISSN 2414-3146

Ethyl 2-(4-methoxyphenyl)-1-methyl-1*H*-benzimidazole-5-carboxylate

S. Naveen,[a] Vasantha Kumar,[b,c] Boja Poojary,[c] Naveen Kumar,[b] Nora Jarrar,[d] N. K. Lokanath[e]* and Ismail Warad[d]*

[a]Institution of Excellence, University of Mysore, Manasagangotri, Mysuru 570 006, India, [b]PG Department of Chemistry, SDM College (Autonomous), Ujire 574 240, India, [c]Department of Chemistry, Mangalore University, Mangaluru 574 199, India, [d]Department of Chemistry, Science College, An-Najah National University, PO Box 7, Nablus, West Bank, Palestinian Territories, and [e]Department of Studies in Physics, University of Mysore, Manasagangotri, Mysuru 570 006, India. *Correspondence e-mail: lokanath@physics.uni-mysore.ac.in, khalil.i@najah.edu

Received 17 March 2017
Accepted 20 March 2017

Edited by D.-J. Xu, Zhejiang University (Yuquan Campus), China

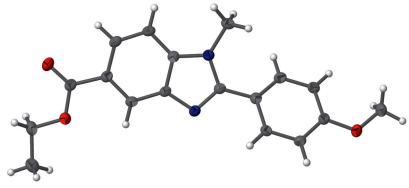
Keywords: crystal structure; benzimidazole; extended conformation.

CCDC reference: 1538919

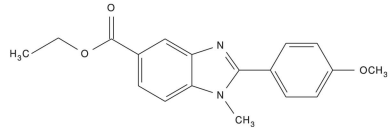
Structural data: full structural data are available from iucrdata.iucr.org

In the title benzimidazole derivative, $C_{18}H_{18}N_2O_3$, the methoxyphenyl ring is twisted with respect to the benzimidazole ring system, making a dihedral angle of 28.81 (5)°. The pendant ethyl chain has an extended conformation. Within the imidazole ring, the C—N single bonds have a partial double-bond character. In the crystal, molecules are linked by weak C—H$\cdots\pi$ interactions and π–π stacking [the centroid-to-centroid distances being 3.6468 (7), 3.7279 (7) and 3.7481 (7) Å].

3D view



Chemical scheme



Structure description

Benzimidazole and its derivatives are found to exhibit various biological activities such as antimicrobial (Göker *et al.*, 2002), anti-inflammatory, antiallergic, antioxidant, anti-tubercular, anticancer, anthelmintic, antiviral and antimalarial. As part of ongoing research on benzimidazoles (Naveen *et al.*, 2016*a*,*b*; Saberi *et al.*, 2009), we report herein on the synthesis and crystal structure of the title compound.

The title molecule, Fig. 1, is non-planar with the methoxyphenyl and the benzimidazole ring system inclined at an angle of 28.81 (5)°. The pendant ethyl chain has an extended conformation, as indicated by the C5—C16—O2—C17 torsion angle of −172.79 (10)°. The imidazole ring is planar, with a maximum deviation of 0.0163 (12) Å for the atom C7. The formal single bonds C1—N1 = 1.3839 (15) Å and C2—N1 = 1.3797 (15) Å have a partial double-bond character, and are significantly shorter than the Csp^2—N bond distance. The methoxy group lies in the plane of the phenyl ring, as indicated by the C15—O1—C12—C13 torsion angle of −2.36 (18)°.

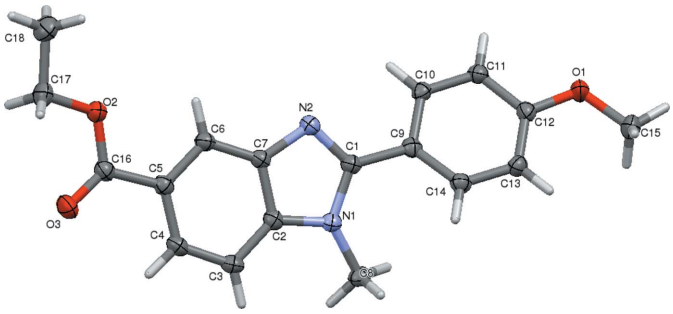


Figure 1
A view of the molecular structure of the title compound, with the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

In the crystal, the molecules are linked by weak C—H···π (Table 1) and π–π stacking [centroid-to-centroid distances = 3.6468 (7), 3.7279 (7) and 3.7481 (7) Å] interactions.

Synthesis and crystallization

Sodium dithionite (3.0 eq) was added to a stirred solution of ethyl 3-nitro-4-(propylamino)benzoate (3.9 mmol) and 4-methoxy benzaldehyde (3.9 mmol) in DMSO (15 ml). The reaction mixture was stirred at 363 K for 3 h. After the completion of reaction [monitored by TLC hexane: ethyl acetate (7: 3, *v*/*v*)], it was poured onto crushed ice. The solid separated was filtered off, washed with water and dried. The product was recrystallized using dimethylformamide to get prismatic brown crystals. Yield 85%, m.p. 507 K.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

The authors are grateful to the Institution of Excellence, Vijnana Bhavana, University of Mysore, India, for providing the single-crystal X-ray diffractometer facility.

References

Bruker (2013). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

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

*Cg*3 is the centroid of the C9–C14 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14···$Cg3^{i}$	0.93	2.81	3.4950 (13)	132

Symmetry code: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, z$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{18}N_2O_3$
M_r	310.34
Crystal system, space group	Orthorhombic, *Pbcn*
Temperature (K)	296
a, b, c (Å)	13.5151 (3), 7.3929 (2), 30.6704 (8)
V (Å^3)	3064.46 (13)
Z	8
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.75
Crystal size (mm)	0.27 × 0.24 × 0.22
Data collection	
Diffractometer	Bruker X8 Proteum
Absorption correction	Multi-scan (*SADABS*; Bruker, 2013)
T_{min}, T_{max}	0.822, 0.852
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10668, 2510, 2422
R_{int}	0.026
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.585
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.034, 0.090, 1.04
No. of reflections	2510
No. of parameters	212
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.16, −0.15

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2008).

Göker, H., Kuş, C., Boykin, D. W., Yildiz, S. & Altanlar, N. (2002). *Bioorg. Med. Chem.* **10**, 2589–2596.
Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
Naveen, S., Kumar, V., Poojary, B., Shivarama Holla, B., Lokanath, N. K. & Abdoh, M. M. M. (2016*a*). *IUCrData*, **1**, x161759.
Naveen, S., Kumar, V., Poojary, B., Vishwanatha, P., Lokanath, N. K. & Abdoh, M. M. M. (2016*b*). *IUCrData*, **1**, x161744.
Saberi, A., Manjunath, H. R., Naveen, S., Prasad, T. N. M., Rangappa, K. S., Sridhar, M. A. & Prasad, J. S. (2009). *Mol. Cryst. Liq. Cryst.* **515**, 199–206.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

full crystallographic data

IUCrData (2017). **2**, x170438 [https://doi.org/10.1107/S2414314617004382]

Ethyl 2-(4-methoxyphenyl)-1-methyl-1*H*-benzimidazole-5-carboxylate

S. Naveen, Vasantha Kumar, Boja Poojary, Naveen Kumar, Nora Jarrar, N. K. Lokanath and Ismail Warad

Ethyl 2-(4-methoxyphenyl)-1-methyl-1*H*-benzimidazole-5-carboxylate

Crystal data

$C_{18}H_{18}N_2O_3$
M_r = 310.34
Orthorhombic, *Pbcn*
Hall symbol: -P 2n 2ab
a = 13.5151 (3) Å
b = 7.3929 (2) Å
c = 30.6704 (8) Å
V = 3064.46 (13) Å^3
Z = 8
F(000) = 1312
D_x = 1.345 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54178 Å
Cell parameters from 2422 reflections
θ = 6.6–64.4°
μ = 0.75 mm^{-1}
T = 296 K
Prism, brown
0.27 × 0.24 × 0.22 mm

Data collection

Bruker X8 Proteum diffractometer
Radiation source: Bruker MicroStar microfocus rotating anode
Helios multilayer optics monochromator
Detector resolution: 18.4 pixels mm^{-1}
φ and *ω* scans
Absorption correction: multi-scan (SADABS; Bruker, 2013)
T_{min} = 0.822, T_{max} = 0.852
10668 measured reflections
2510 independent reflections
2422 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 64.4°, θ_{min} = 6.6°
h = −15→14
k = −8→5
l = −35→28

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.090
S = 1.04
2510 reflections
212 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
$w = 1/[\sigma^2(F_o^2) + (0.048P)^2 + 1.1189P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Extinction correction: SHELXL97 (Sheldrick, 2008), FC*=KFC[1+0.001XFC$^2\Lambda^3$/SIN(2Θ)]$^{-1/4}$
Extinction coefficient: 0.0031 (4)

Special details

Experimental. M.p.: 234 °C; IR (KBr, γmax, cm-1): 3040 (=C-H), 2953 (C-H), 1713 (C=O), 1616 (C=N), 1538 (C=C), 1296 (C-O); 1H NMR (400 MHz, DMSO-d6, δ ppm): 8.53 (s,1H, benzimidazole-H4), 8.02-8.00 (dd, 1H, 8Hz and 2Hz, benzimidazole-H6), 7.65-7.63 (dd, 2H, J = 8 Hz and 2 Hz, 4-methoxyphenyl-H), 7.40 (d, 1H, J = 8 Hz, benzimidazole-H7), 7.04 (d, 2H, J = 8 Hz, 4-methoxyphenyl-H), 4.46-4.40 (q, 2H, J = 7.5 Hz, CH2), 4.03 (s, 3H, CH3), 3.84 (s, 3H, OCH3), 1.32 (t, 3H, J = 7.5 Hz, CH3); MS (m/z): 311.4 (M+1); Anal. calcd. For $C_{18}H_{18}N_2O_3$: C, 69.66; H, 5.85; N, 9.03; Found: C, 69.68; H, 5.87; N, 9.06.

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.08135 (7)	0.56378 (13)	0.71043 (3)	0.0312 (3)
O2	0.11642 (7)	0.08394 (12)	0.35399 (3)	0.0268 (3)
O3	0.27489 (7)	0.06640 (14)	0.33238 (3)	0.0355 (3)
N1	0.30071 (7)	0.35550 (13)	0.52717 (3)	0.0216 (3)
N2	0.13886 (7)	0.32053 (14)	0.51133 (3)	0.0223 (3)
C1	0.20388 (9)	0.36488 (16)	0.54167 (4)	0.0209 (3)
C2	0.29650 (9)	0.29805 (15)	0.48441 (4)	0.0212 (3)
C3	0.37076 (9)	0.26025 (16)	0.45417 (4)	0.0238 (4)
C4	0.33989 (9)	0.20238 (16)	0.41371 (4)	0.0237 (3)
C5	0.23893 (9)	0.18021 (16)	0.40344 (4)	0.0223 (3)
C6	0.16582 (9)	0.21861 (16)	0.43400 (4)	0.0220 (3)
C7	0.19542 (9)	0.27813 (15)	0.47489 (4)	0.0205 (3)
C8	0.39114 (9)	0.41890 (17)	0.54821 (4)	0.0257 (4)
C9	0.17570 (9)	0.41237 (16)	0.58652 (4)	0.0212 (3)
C10	0.08255 (9)	0.48988 (16)	0.59397 (4)	0.0215 (3)
C11	0.05289 (9)	0.53785 (17)	0.63549 (4)	0.0233 (3)
C12	0.11594 (9)	0.50725 (17)	0.67093 (4)	0.0231 (3)
C13	0.20661 (9)	0.42354 (17)	0.66442 (4)	0.0244 (3)
C14	0.23554 (9)	0.37614 (17)	0.62252 (4)	0.0240 (3)
C15	0.14151 (11)	0.5281 (2)	0.74794 (4)	0.0339 (4)
C16	0.21437 (9)	0.10645 (17)	0.35984 (4)	0.0244 (4)
C17	0.08742 (11)	−0.0079 (2)	0.31430 (4)	0.0318 (4)
C18	−0.02236 (11)	−0.0354 (2)	0.31644 (5)	0.0375 (5)
H3	0.43740	0.27340	0.46090	0.0290*
H4	0.38710	0.17720	0.39250	0.0280*
H6	0.09920	0.20480	0.42720	0.0260*
H8A	0.42190	0.32030	0.56340	0.0390*
H8B	0.37530	0.51330	0.56850	0.0390*
H8C	0.43570	0.46490	0.52650	0.0390*
H10	0.04010	0.50930	0.57060	0.0260*

H11	−0.00880	0.59040	0.63990	0.0280*
H13	0.24780	0.39930	0.68800	0.0290*
H14	0.29610	0.31900	0.61840	0.0290*
H15A	0.15260	0.40020	0.75040	0.0510*
H15B	0.10840	0.57100	0.77360	0.0510*
H15C	0.20380	0.58910	0.74490	0.0510*
H17A	0.12100	−0.12340	0.31200	0.0380*
H17B	0.10460	0.06470	0.28910	0.0380*
H18A	−0.03870	−0.10130	0.34240	0.0560*
H18B	−0.04380	−0.10250	0.29140	0.0560*
H18C	−0.05490	0.08010	0.31690	0.0560*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0268 (5)	0.0484 (6)	0.0183 (5)	0.0074 (4)	0.0001 (4)	−0.0012 (4)
O2	0.0244 (5)	0.0332 (5)	0.0229 (5)	0.0015 (4)	−0.0008 (4)	−0.0036 (4)
O3	0.0303 (5)	0.0497 (6)	0.0266 (5)	−0.0012 (4)	0.0074 (4)	−0.0084 (4)
N1	0.0196 (5)	0.0229 (5)	0.0223 (5)	−0.0013 (4)	0.0006 (4)	0.0002 (4)
N2	0.0204 (5)	0.0251 (5)	0.0215 (5)	0.0004 (4)	0.0020 (4)	0.0002 (4)
C1	0.0198 (6)	0.0193 (6)	0.0236 (6)	0.0005 (5)	0.0012 (5)	0.0019 (5)
C2	0.0221 (6)	0.0187 (6)	0.0227 (6)	−0.0004 (5)	0.0012 (5)	0.0017 (5)
C3	0.0178 (6)	0.0248 (6)	0.0288 (7)	−0.0002 (5)	0.0025 (5)	0.0006 (5)
C4	0.0212 (6)	0.0238 (6)	0.0261 (6)	0.0015 (5)	0.0058 (5)	0.0006 (5)
C5	0.0226 (6)	0.0213 (6)	0.0230 (6)	0.0014 (5)	0.0025 (5)	0.0017 (5)
C6	0.0184 (6)	0.0231 (6)	0.0244 (6)	0.0008 (5)	0.0010 (5)	0.0020 (5)
C7	0.0191 (6)	0.0202 (6)	0.0222 (6)	0.0010 (5)	0.0032 (5)	0.0018 (5)
C8	0.0207 (6)	0.0275 (7)	0.0290 (7)	−0.0036 (5)	−0.0024 (5)	0.0022 (5)
C9	0.0220 (6)	0.0191 (6)	0.0224 (6)	−0.0027 (5)	0.0010 (5)	0.0014 (5)
C10	0.0205 (6)	0.0224 (6)	0.0217 (6)	−0.0022 (5)	−0.0020 (5)	0.0012 (5)
C11	0.0189 (6)	0.0261 (6)	0.0250 (6)	0.0006 (5)	0.0013 (5)	0.0006 (5)
C12	0.0229 (6)	0.0264 (6)	0.0201 (6)	−0.0028 (5)	0.0019 (5)	0.0010 (5)
C13	0.0226 (6)	0.0281 (6)	0.0225 (6)	0.0007 (5)	−0.0021 (5)	0.0044 (5)
C14	0.0210 (6)	0.0254 (6)	0.0256 (6)	0.0024 (5)	0.0013 (5)	0.0029 (5)
C15	0.0308 (7)	0.0510 (8)	0.0200 (6)	0.0031 (7)	−0.0026 (5)	−0.0003 (6)
C16	0.0247 (7)	0.0254 (6)	0.0231 (6)	0.0013 (5)	0.0035 (5)	0.0022 (5)
C17	0.0354 (8)	0.0367 (7)	0.0233 (7)	−0.0006 (6)	−0.0031 (6)	−0.0048 (6)
C18	0.0356 (8)	0.0425 (8)	0.0344 (8)	−0.0056 (6)	−0.0051 (6)	−0.0054 (6)

Geometric parameters (Å, º)

O1—C12	1.3641 (15)	C12—C13	1.3873 (17)
O1—C15	1.4332 (16)	C13—C14	1.3882 (17)
O2—C16	1.3462 (15)	C17—C18	1.499 (2)
O2—C17	1.4479 (16)	C3—H3	0.9300
O3—C16	1.2108 (15)	C4—H4	0.9300
N1—C1	1.3839 (15)	C6—H6	0.9300
N1—C2	1.3797 (15)	C8—H8A	0.9600

N1—C8	1.4594 (15)	C8—H8B	0.9600
N2—C1	1.3212 (15)	C8—H8C	0.9600
N2—C7	1.3899 (15)	C10—H10	0.9300
C1—C9	1.4699 (17)	C11—H11	0.9300
C2—C3	1.3948 (17)	C13—H13	0.9300
C2—C7	1.4047 (17)	C14—H14	0.9300
C3—C4	1.3773 (17)	C15—H15A	0.9600
C4—C5	1.4099 (17)	C15—H15B	0.9600
C5—C6	1.3912 (17)	C15—H15C	0.9600
C5—C16	1.4818 (17)	C17—H17A	0.9700
C6—C7	1.3880 (17)	C17—H17B	0.9700
C9—C10	1.4020 (17)	C18—H18A	0.9600
C9—C14	1.3946 (17)	C18—H18B	0.9600
C10—C11	1.3813 (17)	C18—H18C	0.9600
C11—C12	1.3996 (17)		

C12—O1—C15	117.52 (10)	C4—C3—H3	122.00
C16—O2—C17	115.86 (10)	C3—C4—H4	119.00
C1—N1—C2	106.37 (9)	C5—C4—H4	119.00
C1—N1—C8	129.33 (10)	C5—C6—H6	121.00
C2—N1—C8	123.62 (10)	C7—C6—H6	121.00
C1—N2—C7	104.86 (10)	N1—C8—H8A	109.00
N1—C1—N2	112.97 (10)	N1—C8—H8B	109.00
N1—C1—C9	123.90 (11)	N1—C8—H8C	109.00
N2—C1—C9	123.10 (11)	H8A—C8—H8B	110.00
N1—C2—C3	131.61 (11)	H8A—C8—H8C	110.00
N1—C2—C7	105.66 (10)	H8B—C8—H8C	109.00
C3—C2—C7	122.72 (11)	C9—C10—H10	119.00
C2—C3—C4	116.32 (11)	C11—C10—H10	119.00
C3—C4—C5	122.04 (11)	C10—C11—H11	120.00
C4—C5—C6	120.87 (11)	C12—C11—H11	120.00
C4—C5—C16	117.46 (11)	C12—C13—H13	120.00
C6—C5—C16	121.60 (11)	C14—C13—H13	120.00
C5—C6—C7	117.95 (11)	C9—C14—H14	119.00
N2—C7—C2	110.13 (10)	C13—C14—H14	119.00
N2—C7—C6	129.76 (11)	O1—C15—H15A	109.00
C2—C7—C6	120.09 (11)	O1—C15—H15B	109.00
C1—C9—C10	118.87 (11)	O1—C15—H15C	109.00
C1—C9—C14	123.01 (11)	H15A—C15—H15B	110.00
C10—C9—C14	118.05 (11)	H15A—C15—H15C	109.00
C9—C10—C11	121.05 (11)	H15B—C15—H15C	109.00
C10—C11—C12	119.85 (11)	O2—C17—H17A	110.00
O1—C12—C11	115.57 (11)	O2—C17—H17B	110.00
O1—C12—C13	124.56 (11)	C18—C17—H17A	110.00
C11—C12—C13	119.88 (11)	C18—C17—H17B	110.00
C12—C13—C14	119.65 (11)	H17A—C17—H17B	109.00
C9—C14—C13	121.41 (11)	C17—C18—H18A	109.00
O2—C16—O3	122.78 (11)	C17—C18—H18B	110.00

O2—C16—C5	112.71 (10)	C17—C18—H18C	109.00
O3—C16—C5	124.50 (11)	H18A—C18—H18B	109.00
O2—C17—C18	107.14 (11)	H18A—C18—H18C	110.00
C2—C3—H3	122.00	H18B—C18—H18C	109.00
C15—O1—C12—C11	177.32 (11)	N1—C2—C7—C6	−179.07 (10)
C15—O1—C12—C13	−2.36 (18)	C3—C2—C7—N2	178.38 (11)
C17—O2—C16—O3	5.78 (18)	C3—C2—C7—C6	0.00 (18)
C17—O2—C16—C5	−172.79 (10)	C2—C3—C4—C5	−0.76 (17)
C16—O2—C17—C18	174.33 (11)	C3—C4—C5—C6	0.82 (18)
C2—N1—C1—N2	−0.92 (13)	C3—C4—C5—C16	−176.30 (11)
C2—N1—C1—C9	176.89 (11)	C4—C5—C6—C7	−0.41 (17)
C8—N1—C1—N2	169.74 (11)	C16—C5—C6—C7	176.59 (11)
C8—N1—C1—C9	−12.44 (19)	C4—C5—C16—O2	177.52 (10)
C1—N1—C2—C3	−178.03 (12)	C4—C5—C16—O3	−1.02 (19)
C1—N1—C2—C7	0.94 (12)	C6—C5—C16—O2	0.42 (17)
C8—N1—C2—C3	10.64 (19)	C6—C5—C16—O3	−178.11 (12)
C8—N1—C2—C7	−170.39 (10)	C5—C6—C7—N2	−178.00 (11)
C7—N2—C1—N1	0.47 (13)	C5—C6—C7—C2	0.00 (17)
C7—N2—C1—C9	−177.36 (11)	C1—C9—C10—C11	−179.61 (11)
C1—N2—C7—C2	0.16 (13)	C14—C9—C10—C11	3.36 (18)
C1—N2—C7—C6	178.32 (12)	C1—C9—C14—C13	179.78 (12)
N1—C1—C9—C10	153.90 (11)	C10—C9—C14—C13	−3.32 (18)
N1—C1—C9—C14	−29.23 (18)	C9—C10—C11—C12	−0.71 (19)
N2—C1—C9—C10	−28.51 (18)	C10—C11—C12—O1	178.21 (11)
N2—C1—C9—C14	148.37 (12)	C10—C11—C12—C13	−2.09 (19)
N1—C2—C3—C4	179.18 (12)	O1—C12—C13—C14	−178.19 (12)
C7—C2—C3—C4	0.36 (17)	C11—C12—C13—C14	2.14 (19)
N1—C2—C7—N2	−0.70 (13)	C12—C13—C14—C9	0.61 (19)

Hydrogen-bond geometry (Å, º)

Cg3 is the centroid of the C9–C14 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14···*Cg*3^{i}	0.93	2.81	3.4950 (13)	132

Symmetry code: (i) −*x*+1/2, *y*−1/2, *z*.