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

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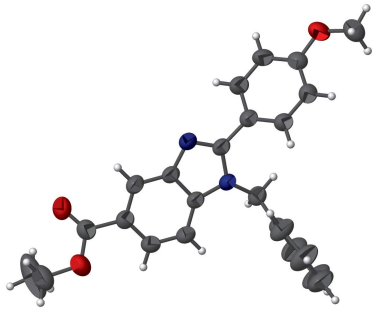
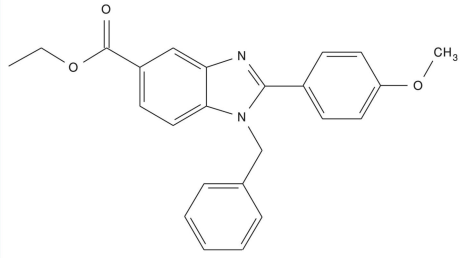
The title benzimidazole derivative, $C_{24}H_{22}N_2O_3$, is T-shaped with the methoxyphenyl and benzyl rings inclined to the imidazole ring system (r.m.s. deviation = 0.009 Å) by 46.73 (10) and 88.88 (15)°, respectively. The phenyl ring and methoxyphenyl rings are inclined at an angle of 82.14 (16)°. In the crystal, weak C—H···O hydrogen bonds link the molecules into [101] *C*(14) chains.

3D view



Chemical scheme



Structure description

Benzimidazole ring systems occur in many marketed drugs such as candesartan and pimobendan. Benzimidazole-5-carboxylates act as anti-HIV agents against hepatitis C virus infections (Zhao *et al.* 2015). As a part of our ongoing research on benzimidazoles (Saberi *et al.* 2009), we report herein on the synthesis and crystal structure of the title compound.

The *ORTEP* of the molecule is shown in Fig. 1. The molecule is T-shaped with the methoxyphenyl (C8–C13) and the benzyl (C19–C24) rings inclined to the imidazole ring system N1/N2/C1–C7 by 46.73 (10) and 88.88 (15)°, respectively, indicating that the benzyl ring is nearly orthogonal to the imidazole ring system. The phenyl ring and the methoxy phenyl rings are inclined at an angle of 82.14 (16)°.

In the crystal, weak C—H···O hydrogen bonds link the molecules into [101] *C*(14) chains (Table 1). The molecules exhibit layered stacking when viewed along the *b* axis (Fig. 2).

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

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14C···O1^{i}	0.96	2.59	3.498 (4)	157

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

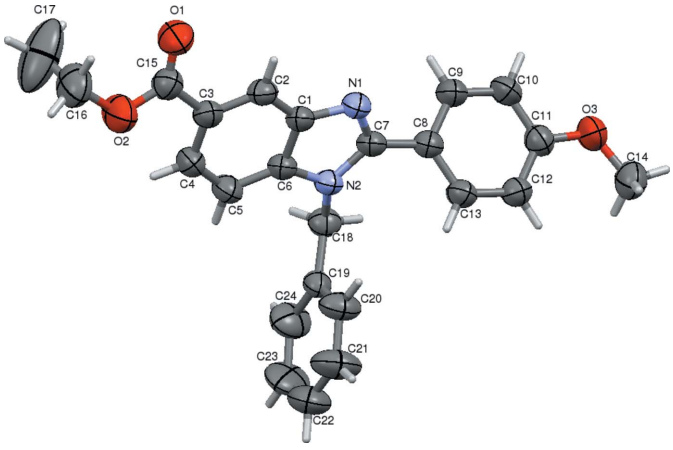


Figure 1
A view of the molecular structure of the title compound, with displacement ellipsoids for non-H atoms drawn at the 50% probability level.

Synthesis and crystallization

Sodium dithionite (3.0 equiv) was added to a stirred solution of ethyl-4-(4-benzylamino)-3-nitrobenzoate (0.01 mol) and 4-methoxybenzaldehyde (0.01 mol) in DMSO (20 ml). The reaction mixture was stirred at 90°C 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 that separated was filtered off, washed with water and dried. The product was recrystallized from dimethylformamide solution to yield colourless prisms; m.p.: 156–158°C.

Refinement

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{24}H_{22}N_2O_3$
M_r	386.44
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, b, c (Å)	10.3178 (11), 10.6067 (11), 10.9071 (12)
α, β, γ (°)	112.306 (3), 104.249 (4), 101.904 (4)
V (Å^3)	1008.81 (19)
Z	2
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.68
Crystal size (mm)	0.28 × 0.25 × 0.22
Data collection	
Diffractometer	Bruker X8 Proteum
Absorption correction	Multi-scan (*SADABS*; Bruker, 2013)
T_{min}, T_{max}	0.832, 0.865
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13401, 3314, 2905
R_{int}	0.043
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.585
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.065, 0.204, 1.05
No. of reflections	3314
No. of parameters	264
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.45, −0.35

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

Acknowledgements

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References

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

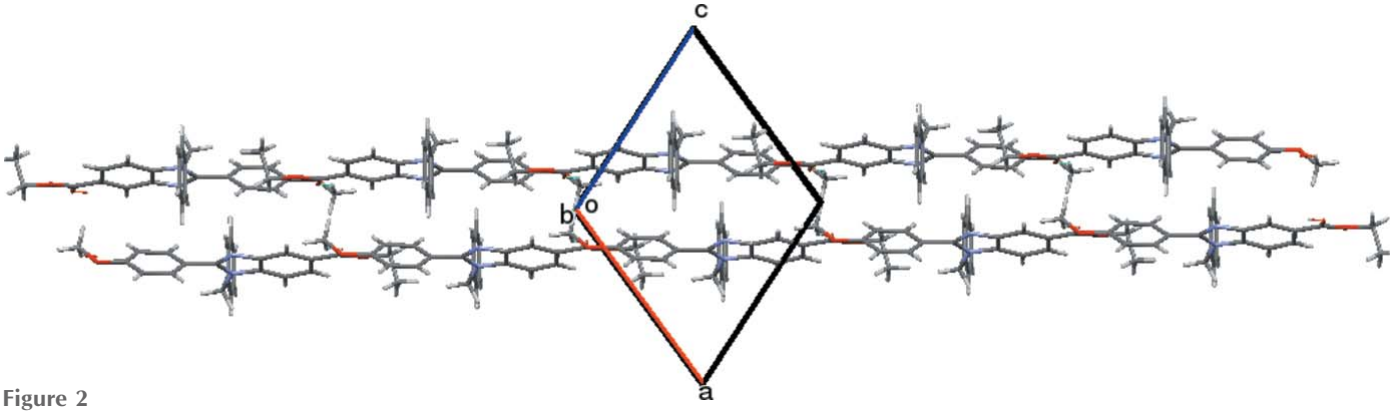

Figure 2
A view along the *b* axis of the title compound, showing layered stacking. The dotted lines represent hydrogen bonds.

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.
Zhao, C., Wang, Y. & Ma, S. (2015). *Eur. J. Med. Chem.* **102**, 188–214.

full crystallographic data

IUCrData (2016). **1**, x161759 [https://doi.org/10.1107/S2414314616017594]

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Crystal data

$C_{24}H_{22}N_2O_3$
M_r = 386.44
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 10.3178 (11) Å
b = 10.6067 (11) Å
c = 10.9071 (12) Å
α = 112.306 (3)°
β = 104.249 (4)°
γ = 101.904 (4)°
V = 1008.81 (19) Å^3
Z = 2
$F(000)$ = 408
D_x = 1.272 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 2905 reflections
θ = 4.5–64.5°
μ = 0.68 mm^{-1}
T = 296 K
Prism, colourless
0.28 × 0.25 × 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} = 0.832, T_{max} = 0.865
13401 measured reflections
3314 independent reflections
2905 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 64.5°, θ_{min} = 4.7°
h = −11→11
k = −12→12
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.204
S = 1.05
3314 reflections
264 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1321P)^2 + 0.249P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Special details

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.
The hydrogen atoms were fixed geometrically (C—H= 0.93–0.96 Å) and allowed to ride on their parent atoms with U_{iso}(H) =1.5U_{eq}(*C*-methyl) and = 1.2U_{eq}(C).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	1.1345 (2)	0.4707 (2)	0.9490 (2)	0.0819 (7)
O2	1.2422 (2)	0.7026 (2)	1.0151 (2)	0.1004 (8)
O3	0.15440 (19)	0.06462 (19)	−0.0631 (2)	0.0761 (6)
N1	0.70029 (18)	0.34906 (19)	0.5025 (2)	0.0541 (6)
N2	0.75013 (18)	0.53336 (17)	0.44821 (18)	0.0479 (5)
C1	0.8274 (2)	0.4539 (2)	0.6035 (2)	0.0478 (6)
C2	0.9192 (2)	0.4567 (2)	0.7220 (2)	0.0523 (7)
C3	1.0411 (2)	0.5752 (2)	0.8052 (2)	0.0537 (7)
C4	1.0716 (2)	0.6898 (2)	0.7699 (3)	0.0612 (7)
C5	0.9822 (2)	0.6887 (2)	0.6530 (3)	0.0593 (7)
C6	0.8595 (2)	0.5695 (2)	0.5706 (2)	0.0475 (6)
C7	0.6583 (2)	0.3990 (2)	0.4119 (2)	0.0489 (6)
C8	0.5275 (2)	0.3191 (2)	0.2854 (2)	0.0515 (7)
C9	0.4973 (3)	0.1723 (2)	0.2028 (3)	0.0652 (8)
C10	0.3729 (3)	0.0916 (3)	0.0883 (3)	0.0710 (8)
C11	0.2729 (2)	0.1544 (3)	0.0531 (2)	0.0589 (7)
C12	0.3010 (2)	0.3007 (2)	0.1350 (2)	0.0581 (7)
C13	0.4272 (2)	0.3818 (2)	0.2499 (2)	0.0559 (7)
C14	0.0398 (3)	0.1163 (3)	−0.0935 (3)	0.0814 (10)
C15	1.1414 (3)	0.5745 (3)	0.9281 (3)	0.0622 (8)
C16	1.3552 (4)	0.7102 (5)	1.1320 (4)	0.1037 (14)
C17	1.4595 (5)	0.6764 (9)	1.0836 (6)	0.181 (3)
C18	0.7560 (2)	0.6083 (2)	0.3608 (2)	0.0549 (7)
C19	0.7436 (2)	0.7562 (2)	0.4225 (2)	0.0496 (6)
C20	0.6656 (3)	0.7919 (3)	0.5065 (3)	0.0737 (10)
C21	0.6474 (5)	0.9258 (3)	0.5525 (4)	0.1012 (15)
C22	0.7078 (4)	1.0245 (3)	0.5153 (5)	0.1011 (15)
C23	0.7836 (4)	0.9912 (4)	0.4318 (6)	0.121 (2)
C24	0.8041 (4)	0.8571 (4)	0.3853 (4)	0.0938 (14)
H2	0.89910	0.38060	0.74480	0.0630*
H4	1.15460	0.76830	0.82740	0.0730*
H5	1.00300	0.76460	0.63000	0.0710*
H9	0.56230	0.12810	0.22530	0.0780*
H10	0.35520	−0.00630	0.03370	0.0850*

H12	0.23530	0.34430	0.11290	0.0700*
H13	0.44520	0.47980	0.30430	0.0670*
H14A	0.00560	0.14070	−0.01620	0.1220*
H14B	−0.03540	0.04250	−0.17890	0.1220*
H14C	0.07180	0.20060	−0.10620	0.1220*
H16A	1.39300	0.80690	1.21060	0.1240*
H16B	1.31810	0.64270	1.16510	0.1240*
H17A	1.42420	0.57690	1.01350	0.2710*
H17B	1.53920	0.69110	1.16130	0.2710*
H17C	1.48860	0.73720	1.04200	0.2710*
H18A	0.68000	0.54940	0.26930	0.0660*
H18B	0.84510	0.61700	0.34470	0.0660*
H20	0.62380	0.72530	0.53340	0.0880*
H21	0.59330	0.94790	0.60940	0.1210*
H22	0.69670	1.11490	0.54750	0.1220*
H23	0.82320	1.05820	0.40430	0.1450*
H24	0.85890	0.83630	0.32900	0.1120*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0830 (12)	0.0793 (13)	0.0802 (12)	0.0231 (10)	0.0081 (10)	0.0481 (11)
O2	0.0881 (14)	0.0772 (13)	0.0923 (14)	0.0109 (11)	−0.0177 (11)	0.0349 (12)
O3	0.0630 (10)	0.0582 (10)	0.0732 (11)	0.0116 (8)	0.0016 (8)	0.0147 (9)
N1	0.0513 (10)	0.0429 (9)	0.0650 (11)	0.0133 (8)	0.0130 (8)	0.0274 (8)
N2	0.0523 (9)	0.0384 (9)	0.0529 (10)	0.0154 (7)	0.0155 (8)	0.0226 (7)
C1	0.0482 (10)	0.0389 (10)	0.0580 (12)	0.0179 (8)	0.0192 (9)	0.0218 (9)
C2	0.0554 (11)	0.0470 (11)	0.0629 (12)	0.0224 (9)	0.0225 (10)	0.0298 (10)
C3	0.0544 (12)	0.0482 (12)	0.0581 (12)	0.0224 (10)	0.0182 (10)	0.0223 (10)
C4	0.0538 (12)	0.0457 (12)	0.0701 (14)	0.0097 (9)	0.0103 (10)	0.0232 (11)
C5	0.0604 (12)	0.0443 (12)	0.0683 (14)	0.0110 (10)	0.0162 (11)	0.0283 (11)
C6	0.0505 (11)	0.0395 (10)	0.0539 (11)	0.0176 (8)	0.0182 (9)	0.0215 (9)
C7	0.0516 (11)	0.0397 (10)	0.0569 (12)	0.0188 (9)	0.0189 (9)	0.0220 (9)
C8	0.0533 (11)	0.0433 (11)	0.0578 (12)	0.0169 (9)	0.0183 (9)	0.0236 (10)
C9	0.0602 (13)	0.0473 (13)	0.0771 (15)	0.0215 (10)	0.0130 (12)	0.0228 (12)
C10	0.0675 (14)	0.0408 (12)	0.0777 (16)	0.0147 (11)	0.0082 (12)	0.0129 (11)
C11	0.0571 (12)	0.0510 (12)	0.0569 (12)	0.0114 (10)	0.0144 (10)	0.0200 (10)
C12	0.0576 (12)	0.0534 (13)	0.0616 (13)	0.0227 (10)	0.0166 (10)	0.0251 (11)
C13	0.0592 (12)	0.0434 (11)	0.0572 (12)	0.0185 (10)	0.0148 (10)	0.0180 (10)
C14	0.0644 (15)	0.0829 (19)	0.0781 (17)	0.0157 (13)	0.0071 (13)	0.0339 (15)
C15	0.0599 (13)	0.0604 (14)	0.0596 (13)	0.0218 (11)	0.0144 (11)	0.0242 (12)
C16	0.085 (2)	0.110 (3)	0.092 (2)	0.0154 (19)	−0.0024 (18)	0.052 (2)
C17	0.101 (3)	0.354 (9)	0.128 (4)	0.081 (4)	0.035 (3)	0.151 (5)
C18	0.0626 (12)	0.0553 (13)	0.0558 (12)	0.0217 (10)	0.0252 (10)	0.0307 (10)
C19	0.0471 (10)	0.0444 (11)	0.0572 (12)	0.0109 (8)	0.0123 (9)	0.0293 (10)
C20	0.103 (2)	0.0551 (14)	0.0897 (18)	0.0356 (14)	0.0527 (16)	0.0433 (13)
C21	0.149 (3)	0.0676 (18)	0.122 (3)	0.061 (2)	0.073 (2)	0.0500 (19)
C22	0.112 (3)	0.0550 (17)	0.140 (3)	0.0331 (17)	0.038 (2)	0.0497 (19)

C23	0.118 (3)	0.079 (2)	0.205 (5)	0.026 (2)	0.066 (3)	0.103 (3)
C24	0.096 (2)	0.083 (2)	0.143 (3)	0.0294 (16)	0.067 (2)	0.077 (2)

Geometric parameters (Å, º)

O1—C15	1.198 (4)	C19—C24	1.371 (5)
O2—C15	1.334 (4)	C20—C21	1.386 (5)
O2—C16	1.464 (5)	C21—C22	1.352 (6)
O3—C11	1.360 (3)	C22—C23	1.337 (7)
O3—C14	1.422 (4)	C23—C24	1.398 (7)
N1—C1	1.388 (3)	C2—H2	0.9300
N1—C7	1.314 (3)	C4—H4	0.9300
N2—C6	1.376 (3)	C5—H5	0.9300
N2—C7	1.384 (3)	C9—H9	0.9300
N2—C18	1.459 (3)	C10—H10	0.9300
C1—C2	1.388 (3)	C12—H12	0.9300
C1—C6	1.402 (3)	C13—H13	0.9300
C2—C3	1.380 (3)	C14—H14A	0.9600
C3—C4	1.408 (3)	C14—H14B	0.9600
C3—C15	1.482 (4)	C14—H14C	0.9600
C4—C5	1.372 (4)	C16—H16A	0.9700
C5—C6	1.388 (3)	C16—H16B	0.9700
C7—C8	1.472 (3)	C17—H17A	0.9600
C8—C9	1.389 (3)	C17—H17B	0.9600
C8—C13	1.395 (3)	C17—H17C	0.9600
C9—C10	1.373 (4)	C18—H18A	0.9700
C10—C11	1.392 (4)	C18—H18B	0.9700
C11—C12	1.387 (4)	C20—H20	0.9300
C12—C13	1.387 (3)	C21—H21	0.9300
C16—C17	1.364 (7)	C22—H22	0.9300
C18—C19	1.501 (3)	C23—H23	0.9300
C19—C20	1.362 (4)	C24—H24	0.9300
C15—O2—C16	117.5 (3)	C3—C2—H2	121.00
C11—O3—C14	118.6 (2)	C3—C4—H4	119.00
C1—N1—C7	105.3 (2)	C5—C4—H4	119.00
C6—N2—C7	106.36 (18)	C4—C5—H5	121.00
C6—N2—C18	123.52 (19)	C6—C5—H5	121.00
C7—N2—C18	128.33 (17)	C8—C9—H9	120.00
N1—C1—C2	130.1 (2)	C10—C9—H9	120.00
N1—C1—C6	109.81 (18)	C9—C10—H10	120.00
C2—C1—C6	120.1 (2)	C11—C10—H10	120.00
C1—C2—C3	118.4 (2)	C11—C12—H12	120.00
C2—C3—C4	120.7 (2)	C13—C12—H12	120.00
C2—C3—C15	118.0 (2)	C8—C13—H13	119.00
C4—C3—C15	121.3 (2)	C12—C13—H13	119.00
C3—C4—C5	121.8 (2)	O3—C14—H14A	110.00
C4—C5—C6	117.1 (2)	O3—C14—H14B	109.00

N2—C6—C1	105.79 (18)	O3—C14—H14C	109.00
N2—C6—C5	132.2 (2)	H14A—C14—H14B	109.00
C1—C6—C5	122.1 (2)	H14A—C14—H14C	109.00
N1—C7—N2	112.80 (18)	H14B—C14—H14C	109.00
N1—C7—C8	123.1 (2)	O2—C16—H16A	110.00
N2—C7—C8	124.14 (19)	O2—C16—H16B	110.00
C7—C8—C9	118.8 (2)	C17—C16—H16A	110.00
C7—C8—C13	122.90 (19)	C17—C16—H16B	110.00
C9—C8—C13	118.2 (2)	H16A—C16—H16B	108.00
C8—C9—C10	120.9 (3)	C16—C17—H17A	109.00
C9—C10—C11	120.9 (3)	C16—C17—H17B	109.00
O3—C11—C10	115.8 (3)	C16—C17—H17C	110.00
O3—C11—C12	125.2 (2)	H17A—C17—H17B	109.00
C10—C11—C12	119.0 (2)	H17A—C17—H17C	110.00
C11—C12—C13	119.9 (2)	H17B—C17—H17C	109.00
C8—C13—C12	121.2 (2)	N2—C18—H18A	109.00
O1—C15—O2	122.6 (3)	N2—C18—H18B	109.00
O1—C15—C3	124.3 (3)	C19—C18—H18A	108.00
O2—C15—C3	113.1 (3)	C19—C18—H18B	109.00
O2—C16—C17	108.2 (4)	H18A—C18—H18B	108.00
N2—C18—C19	114.94 (17)	C19—C20—H20	119.00
C18—C19—C20	122.7 (2)	C21—C20—H20	119.00
C18—C19—C24	119.2 (2)	C20—C21—H21	120.00
C20—C19—C24	118.0 (3)	C22—C21—H21	120.00
C19—C20—C21	121.1 (3)	C21—C22—H22	120.00
C20—C21—C22	120.4 (4)	C23—C22—H22	120.00
C21—C22—C23	119.5 (4)	C22—C23—H23	119.00
C22—C23—C24	120.9 (4)	C24—C23—H23	120.00
C19—C24—C23	120.1 (4)	C19—C24—H24	120.00
C1—C2—H2	121.00	C23—C24—H24	120.00

C16—O2—C15—O1	6.0 (4)	C2—C3—C15—O2	−169.0 (2)
C16—O2—C15—C3	−173.9 (3)	C4—C3—C15—O1	−166.1 (3)
C15—O2—C16—C17	87.3 (6)	C4—C3—C15—O2	13.8 (4)
C14—O3—C11—C10	171.4 (3)	C3—C4—C5—C6	0.2 (4)
C14—O3—C11—C12	−9.7 (4)	C4—C5—C6—N2	−179.1 (2)
C7—N1—C1—C2	−178.7 (2)	C4—C5—C6—C1	−0.5 (3)
C7—N1—C1—C6	0.5 (2)	N1—C7—C8—C9	−44.3 (3)
C1—N1—C7—N2	−0.8 (2)	N1—C7—C8—C13	131.1 (2)
C1—N1—C7—C8	178.96 (19)	N2—C7—C8—C9	135.4 (2)
C7—N2—C6—C1	−0.5 (2)	N2—C7—C8—C13	−49.2 (3)
C7—N2—C6—C5	178.4 (2)	C7—C8—C9—C10	176.4 (2)
C18—N2—C6—C1	−166.32 (19)	C13—C8—C9—C10	0.8 (4)
C18—N2—C6—C5	12.5 (4)	C7—C8—C13—C12	−175.8 (2)
C6—N2—C7—N1	0.8 (2)	C9—C8—C13—C12	−0.4 (3)
C6—N2—C7—C8	−179.0 (2)	C8—C9—C10—C11	−0.9 (4)
C18—N2—C7—N1	165.8 (2)	C9—C10—C11—O3	179.4 (3)
C18—N2—C7—C8	−14.0 (3)	C9—C10—C11—C12	0.5 (4)

C6—N2—C18—C19	−73.5 (3)	O3—C11—C12—C13	−178.8 (2)
C7—N2—C18—C19	123.9 (2)	C10—C11—C12—C13	0.0 (4)
N1—C1—C2—C3	179.3 (2)	C11—C12—C13—C8	0.0 (3)
C6—C1—C2—C3	0.1 (3)	N2—C18—C19—C20	−31.9 (3)
N1—C1—C6—N2	0.0 (2)	N2—C18—C19—C24	153.0 (3)
N1—C1—C6—C5	−179.0 (2)	C18—C19—C20—C21	−174.9 (3)
C2—C1—C6—N2	179.32 (19)	C24—C19—C20—C21	0.3 (4)
C2—C1—C6—C5	0.3 (3)	C18—C19—C24—C23	174.5 (3)
C1—C2—C3—C4	−0.4 (3)	C20—C19—C24—C23	−0.8 (5)
C1—C2—C3—C15	−177.5 (2)	C19—C20—C21—C22	−0.4 (6)
C2—C3—C4—C5	0.2 (4)	C20—C21—C22—C23	1.0 (7)
C15—C3—C4—C5	177.3 (2)	C21—C22—C23—C24	−1.6 (7)
C2—C3—C15—O1	11.0 (4)	C22—C23—C24—C19	1.5 (7)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14*C*···O1^{i}	0.96	2.59	3.498 (4)	157

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