



IUCrData

ISSN 2414-3146

Ethyl 1-(4-fluorobenzyl)-2-(4-methoxyphenyl)-1*H*-benzo[*d*]imidazole-5-carboxylate

S. Naveen,^a Vasantha Kumar,^{b,c} Boja Poojary,^c P. Vishwanatha,^b N. K. Lokanath^d and M. M. M. Abdoh^{e*}

^aInstitution of Excellence, University of Mysore, Manasagangotri, Mysuru 570 006, India, ^bPG Department of Chemistry, SDM College (Autonomous), Ujire 574 240, India, ^cDepartment of Chemistry, Mangalore University, Mangaluru 574 199, India, ^dDepartment of Studies in Physics, University of Mysore, Manasagangotri, Mysuru 570 006, India, and ^eDepartment of Physics, Science College, An-Najah National University, PO Box 7, Nablus, West Bank, Palestinian Territories. *Correspondence e-mail: muneer@najah.edu

Received 28 October 2016

Accepted 31 October 2016

Edited by H. Stoeckli-Evans, University of Neuchâtel, Switzerland

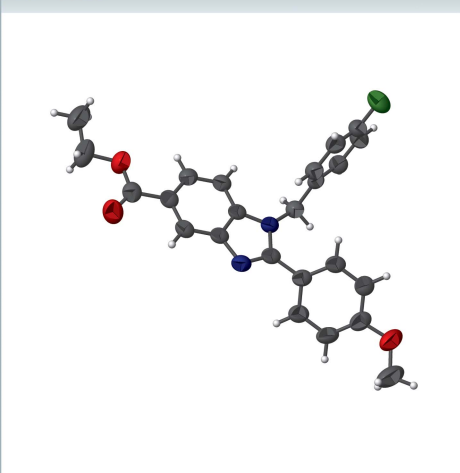
Keywords: crystal structure; benzoimidazole; methoxyphenyl; fluorobenzyl; C—H...O hydrogen bonds.

CCDC reference: 1513685

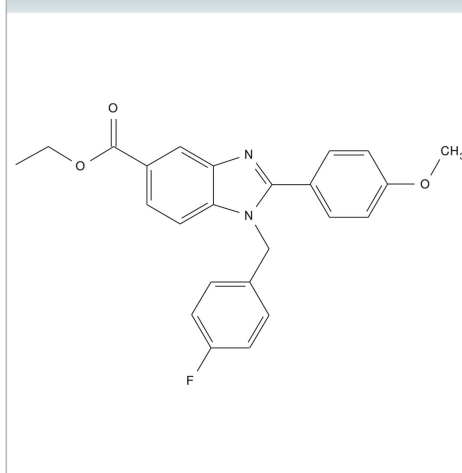
Structural data: full structural data are available from iucrdata.iucr.org

The title benzoimidazole derivative, C₂₄H₂₁FN₂O₃, is T-shaped, with the methoxyphenyl and fluorobenzyl rings inclined to the benzoimidazole ring system by 40.91 (8) and 86.04 (8)°, respectively, indicating that the fluorobenzyl ring system is nearly orthogonal to the benzoimidazole ring system. The fluorobenzyl and methoxyphenyl rings are inclined to one another by 78.90 (10)°. In the crystal, molecules are linked *via* two pairs of C—H...O hydrogen bonds, forming inversion dimers with *R*₂²(28) and *R*₂²(22) ring motifs. As a result of these hydrogen bonds, ribbons propagating along [010] are formed.

3D view



Chemical scheme



Structure description

Benzoimidazole-based compounds possess diverse biological activities such as anti-cancer, antibacterial, antifungal (Venkatesan, 1998), antihelmintic, anti-inflammatory, antihistaminic and proton-pump inhibitor (Veerakumari & Munuswamy, 2000). In our recent work (Madankumar *et al.*, 2016), we have reported on the crystal structures of different benzoimidazoles with varying substitution at positions 1 and 2. Based upon these observations, it was found worth to synthesize some 1,2-disubstituted benzoimidazole-5-carboxylates by using a 'one-pot' nitro-reductive cyclization method and we report herein on the synthesis and crystal structure of the title compound.

The molecular structure is shown in Fig. 1. The molecule is T-shaped with the methoxyphenyl (C11–C16) and fluorobenzyl (C19–C24) rings inclined to the benzoimidazole ring system (N1/N2/C1–C7) by 40.91 (8) and 86.04 (8)°, respectively, indicating that the

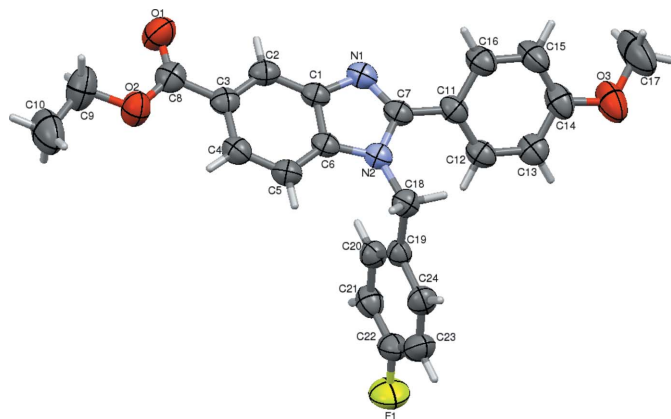


Figure 1
A view of the molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

fluorobenzyl ring is almost orthogonal to the benzimidazole ring system. The fluorobenzyl and methoxyphenyl rings are inclined to one another by $78.9(1)^\circ$. The benzimidazole ring is, as expected, almost planar, with the maximum deviation being $0.024(2)$ Å for atom N1. The methoxy group lies in the plane of the benzene ring and is in a *-synclinal* conformation as indicated by the value of $-17.0(4)^\circ$ for torsion angle C15—C14—O3—C17. The mean plane of the ethyl carboxylate group (O1/O2/C8—C10) is inclined to the benzimidazole ring by $4.53(12)^\circ$.

In the crystal, molecules are linked *via* two pairs of C—H...O hydrogen bonds, forming inversion dimers with $R_2^2(28)$ and $R_2^2(22)$ ring motifs. As a result of these hydrogen bonds, ribbons propagating along [010] are formed (Table 1 and Fig. 2). There are no other significant intermolecular interactions present.

Synthesis and crystallization

Sodium dithionite (3.0 equiv) was added to a stirred solution of ethyl-4-(4-fluorobenzylamino)-3-nitrobenzoate (0.01 mol) and 4-methoxybenzaldehyde (0.01 mol) in DMSO (20 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

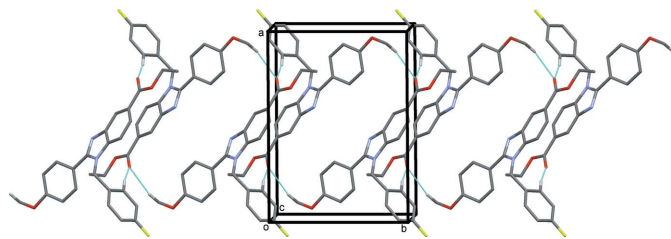


Figure 2
A view along the *c* axis of the crystal packing of the title compound. Hydrogen bonds are shown as dashed lines (see Table 1) and, for clarity, only H atoms H17C and H20 have been included.

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

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C17—H17C...O1 ⁱ	0.96	2.43	3.356 (4)	163
C20—H20...O1 ⁱⁱ	0.93	2.45	3.324 (2)	156

Symmetry codes: (i) $-x + 1, -y + 1, -z + 1$; (ii) $-x + 1, -y, -z + 1$.

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₂₄ H ₂₁ FN ₂ O ₃
<i>M_r</i>	404.43
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>n</i>
Temperature (K)	296
<i>a</i> , <i>b</i> , <i>c</i> (Å)	13.5156 (10), 9.5906 (8), 16.1315 (13)
β (°)	101.409 (3)
<i>V</i> (Å ³)	2049.7 (3)
<i>Z</i>	4
Radiation type	Cu <i>K</i> α
μ (mm ⁻¹)	0.77
Crystal size (mm)	0.29 × 0.27 × 0.24
Data collection	
Diffractometer	Bruker X8 Proteum
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2013)
<i>T_{min}</i> , <i>T_{max}</i>	0.808, 0.837
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	12703, 3318, 2930
<i>R_{int}</i>	0.053
(sin θ/λ) _{max} (Å ⁻¹)	0.584
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.062, 0.182, 1.05
No. of reflections	3318
No. of parameters	274
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	0.21, -0.22

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008) and *PLATON* (Spek, 2009).

that separated was filtered off, washed with water and dried. The product was recrystallized using DMF as the solvent to yield colourless block-like crystals (m.p. 343–345 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.
 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.

- Madankumar, S., Vasantha, K., Boja, P., Byrappa, K. & Warad, I. (2016). *IUCr Data* **1**, x161124.
- Sheldrick, G. M. (2008). *Acta Cryst. A* **64**, 112–122.
- Spek, A. L. (2009). *Acta Cryst. D* **65**, 148–155.
- Veerakumari, L. & Munuswamy, N. (2000). *Vet. Parasitol.* **91**, 129–140.
- Venkatesan, P. (1998). *J. Antimic. Chemoth.* **41**, 145–147.

full crystallographic data

IUCrData (2016). **1**, x161744 [https://doi.org/10.1107/S2414314616017442]

Ethyl 1-(4-fluorobenzyl)-2-(4-methoxyphenyl)-1*H*-benzo[*d*]imidazole-5-carboxylate

S. Naveen, Vasantha Kumar, Boja Poojary, P. Vishwanatha, N. K. Lokanath and M. M. M. Abdoh

Ethyl 1-(4-fluorobenzyl)-2-(4-methoxyphenyl)-1*H*-benzo[*d*]imidazole-5-carboxylate

Crystal data

C₂₄H₂₁FN₂O₃

M_r = 404.43

Monoclinic, *P*2₁/*n*

Hall symbol: -*P* 2₁*n*

a = 13.5156 (10) Å

b = 9.5906 (8) Å

c = 16.1315 (13) Å

β = 101.409 (3)°

V = 2049.7 (3) Å³

Z = 4

F(000) = 848

D_x = 1.311 Mg m⁻³

Cu *K*α radiation, λ = 1.54178 Å

Cell parameters from 2930 reflections

θ = 4.8–64.2°

μ = 0.77 mm⁻¹

T = 296 K

Block, colourless

0.29 × 0.27 × 0.24 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} = 0.808, *T_{max}* = 0.837

12703 measured reflections

3318 independent reflections

2930 reflections with *I* > 2σ(*I*)

R_{int} = 0.053

θ_{max} = 64.2°, θ_{min} = 4.8°

h = -15→15

k = -9→10

l = -17→18

Refinement

Refinement on *F*²

Least-squares matrix: full

R[*F*² > 2σ(*F*²)] = 0.062

wR(*F*²) = 0.182

S = 1.05

3318 reflections

274 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/[σ²(*F_o*²) + (0.1193*P*)² + 0.3084*P*]

where *P* = (*F_o*² + 2*F_c*²)/3

(Δ/σ)_{max} < 0.001

Δρ_{max} = 0.21 e Å⁻³

Δρ_{min} = -0.22 e Å⁻³

Extinction correction: SHELXL97 (Sheldrick,
2008), *FC** = KFC[1 + 0.001XFC²Λ³/SIN(2Θ)]^{-1/4}

Extinction coefficient: 0.0054 (17)

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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
F1	1.07749 (10)	-0.11559 (17)	0.77837 (11)	0.0973 (6)
O1	0.26807 (12)	-0.0335 (2)	0.51786 (10)	0.0797 (6)
O2	0.31003 (11)	-0.14020 (17)	0.64310 (10)	0.0721 (6)
O3	0.94650 (14)	0.72073 (18)	0.50713 (14)	0.0922 (7)
N1	0.58231 (12)	0.29661 (16)	0.53285 (10)	0.0538 (5)
N2	0.68142 (11)	0.25854 (15)	0.66019 (9)	0.0485 (5)
C1	0.53828 (13)	0.19655 (19)	0.57612 (11)	0.0480 (6)
C2	0.44881 (14)	0.1219 (2)	0.55256 (12)	0.0527 (6)
C3	0.42179 (14)	0.0283 (2)	0.60977 (12)	0.0518 (6)
C4	0.48318 (14)	0.0107 (2)	0.69070 (12)	0.0551 (6)
C5	0.57209 (14)	0.0826 (2)	0.71444 (12)	0.0535 (6)
C6	0.59874 (13)	0.17340 (18)	0.65591 (11)	0.0471 (5)
C7	0.66709 (13)	0.33072 (18)	0.58400 (11)	0.0496 (6)
C8	0.32629 (15)	-0.0496 (2)	0.58441 (13)	0.0593 (7)
C9	0.2175 (2)	-0.2203 (3)	0.62499 (19)	0.0911 (10)
C10	0.2212 (3)	-0.3276 (4)	0.6906 (3)	0.1180 (16)
C11	0.73916 (14)	0.43352 (18)	0.56416 (11)	0.0510 (6)
C12	0.84343 (15)	0.4129 (2)	0.58535 (12)	0.0544 (6)
C13	0.90954 (16)	0.5105 (2)	0.56507 (13)	0.0599 (7)
C14	0.87388 (18)	0.6299 (2)	0.52271 (15)	0.0660 (8)
C15	0.77114 (18)	0.6523 (2)	0.49977 (16)	0.0714 (8)
C16	0.70457 (16)	0.5549 (2)	0.52076 (14)	0.0626 (7)
C17	0.9192 (3)	0.8263 (4)	0.4464 (3)	0.1321 (18)
C18	0.76049 (14)	0.2723 (2)	0.73505 (11)	0.0510 (6)
C19	0.84310 (13)	0.16391 (18)	0.74350 (10)	0.0454 (5)
C20	0.84912 (14)	0.06472 (19)	0.68282 (12)	0.0510 (6)
C21	0.92827 (15)	-0.0298 (2)	0.69431 (14)	0.0597 (7)
C22	1.00001 (15)	-0.0228 (2)	0.76717 (15)	0.0642 (7)
C23	0.99693 (16)	0.0737 (3)	0.82863 (14)	0.0683 (8)
C24	0.91817 (15)	0.1667 (2)	0.81640 (12)	0.0578 (6)
H2	0.40790	0.13460	0.49950	0.0630*
H4	0.46300	-0.05090	0.72870	0.0660*
H5	0.61270	0.07070	0.76760	0.0640*
H9A	0.21030	-0.26400	0.56990	0.1100*
H9B	0.16000	-0.15950	0.62440	0.1100*

H10A	0.27220	-0.39500	0.68560	0.1770*
H10B	0.15680	-0.37310	0.68360	0.1770*
H10C	0.23690	-0.28470	0.74540	0.1770*
H12	0.86860	0.33200	0.61360	0.0650*
H13	0.97870	0.49520	0.58020	0.0720*
H15	0.74670	0.73260	0.47030	0.0860*
H16	0.63550	0.57090	0.50550	0.0750*
H17A	0.88370	0.78580	0.39460	0.1980*
H17B	0.97890	0.87230	0.43660	0.1980*
H17C	0.87650	0.89270	0.46670	0.1980*
H18A	0.73000	0.26730	0.78460	0.0610*
H18B	0.79080	0.36390	0.73450	0.0610*
H20	0.79970	0.06120	0.63380	0.0610*
H21	0.93260	-0.09660	0.65340	0.0720*
H23	1.04670	0.07640	0.87750	0.0820*
H24	0.91490	0.23320	0.85780	0.0690*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0674 (9)	0.0911 (10)	0.1323 (14)	0.0300 (7)	0.0171 (8)	0.0145 (9)
O1	0.0667 (10)	0.0970 (13)	0.0703 (10)	-0.0099 (8)	0.0012 (8)	-0.0012 (9)
O2	0.0679 (9)	0.0779 (11)	0.0722 (10)	-0.0165 (7)	0.0182 (7)	-0.0008 (8)
O3	0.0903 (12)	0.0650 (10)	0.1366 (16)	-0.0022 (8)	0.0599 (12)	0.0180 (10)
N1	0.0593 (9)	0.0516 (9)	0.0509 (9)	0.0078 (7)	0.0119 (7)	0.0079 (7)
N2	0.0508 (8)	0.0460 (8)	0.0488 (8)	0.0047 (6)	0.0099 (6)	0.0033 (6)
C1	0.0512 (9)	0.0450 (10)	0.0482 (10)	0.0096 (7)	0.0107 (7)	0.0028 (7)
C2	0.0518 (10)	0.0554 (11)	0.0500 (10)	0.0109 (8)	0.0080 (8)	0.0000 (8)
C3	0.0510 (10)	0.0504 (11)	0.0549 (10)	0.0083 (8)	0.0125 (8)	-0.0029 (8)
C4	0.0581 (11)	0.0520 (11)	0.0575 (11)	0.0054 (8)	0.0173 (8)	0.0065 (8)
C5	0.0552 (10)	0.0539 (11)	0.0502 (10)	0.0062 (8)	0.0077 (8)	0.0056 (8)
C6	0.0504 (9)	0.0420 (9)	0.0494 (9)	0.0094 (7)	0.0111 (7)	0.0025 (7)
C7	0.0552 (10)	0.0449 (10)	0.0498 (10)	0.0103 (8)	0.0133 (8)	0.0030 (8)
C8	0.0572 (11)	0.0607 (12)	0.0620 (12)	0.0036 (9)	0.0168 (9)	-0.0074 (10)
C9	0.0832 (16)	0.103 (2)	0.0922 (18)	-0.0344 (15)	0.0297 (13)	-0.0184 (16)
C10	0.095 (2)	0.092 (2)	0.180 (4)	-0.0134 (16)	0.059 (2)	0.023 (2)
C11	0.0621 (11)	0.0441 (10)	0.0493 (10)	0.0055 (8)	0.0168 (8)	0.0009 (8)
C12	0.0632 (11)	0.0503 (11)	0.0527 (10)	0.0091 (8)	0.0190 (8)	0.0049 (8)
C13	0.0608 (11)	0.0603 (12)	0.0631 (12)	0.0049 (9)	0.0235 (9)	-0.0010 (9)
C14	0.0791 (14)	0.0505 (11)	0.0784 (14)	0.0011 (10)	0.0397 (11)	0.0018 (10)
C15	0.0807 (15)	0.0510 (12)	0.0899 (16)	0.0130 (10)	0.0346 (12)	0.0197 (11)
C16	0.0649 (12)	0.0540 (12)	0.0722 (13)	0.0103 (9)	0.0213 (10)	0.0085 (10)
C17	0.128 (3)	0.092 (2)	0.198 (4)	0.0054 (19)	0.085 (3)	0.060 (2)
C18	0.0565 (10)	0.0497 (10)	0.0468 (10)	0.0010 (8)	0.0101 (8)	-0.0033 (8)
C19	0.0493 (9)	0.0438 (9)	0.0436 (9)	-0.0048 (7)	0.0107 (7)	0.0038 (7)
C20	0.0546 (10)	0.0493 (10)	0.0487 (10)	-0.0017 (8)	0.0093 (8)	-0.0001 (8)
C21	0.0637 (12)	0.0488 (11)	0.0708 (13)	0.0004 (9)	0.0236 (10)	-0.0012 (9)
C22	0.0509 (11)	0.0601 (12)	0.0816 (14)	0.0069 (9)	0.0135 (10)	0.0170 (11)

C23	0.0578 (11)	0.0785 (15)	0.0630 (13)	0.0005 (10)	-0.0018 (9)	0.0097 (11)
C24	0.0632 (11)	0.0603 (12)	0.0477 (10)	-0.0039 (9)	0.0059 (8)	-0.0015 (9)

Geometric parameters (Å, °)

F1—C22	1.359 (3)	C19—C20	1.379 (2)
O1—C8	1.209 (3)	C19—C24	1.393 (3)
O2—C8	1.335 (3)	C20—C21	1.386 (3)
O2—C9	1.447 (3)	C21—C22	1.369 (3)
O3—C14	1.372 (3)	C22—C23	1.363 (3)
O3—C17	1.406 (5)	C23—C24	1.373 (3)
N1—C1	1.388 (2)	C2—H2	0.9300
N1—C7	1.314 (2)	C4—H4	0.9300
N2—C6	1.375 (2)	C5—H5	0.9300
N2—C7	1.390 (2)	C9—H9A	0.9700
N2—C18	1.452 (2)	C9—H9B	0.9700
C1—C2	1.392 (3)	C10—H10A	0.9600
C1—C6	1.399 (2)	C10—H10B	0.9600
C2—C3	1.387 (3)	C10—H10C	0.9600
C3—C4	1.412 (3)	C12—H12	0.9300
C3—C8	1.477 (3)	C13—H13	0.9300
C4—C5	1.373 (3)	C15—H15	0.9300
C5—C6	1.384 (3)	C16—H16	0.9300
C7—C11	1.465 (3)	C17—H17A	0.9600
C9—C10	1.470 (5)	C17—H17B	0.9600
C11—C12	1.397 (3)	C17—H17C	0.9600
C11—C16	1.391 (3)	C18—H18A	0.9700
C12—C13	1.377 (3)	C18—H18B	0.9700
C13—C14	1.371 (3)	C20—H20	0.9300
C14—C15	1.381 (3)	C21—H21	0.9300
C15—C16	1.385 (3)	C23—H23	0.9300
C18—C19	1.512 (3)	C24—H24	0.9300
C8—O2—C9	117.34 (18)	C19—C24—C23	121.56 (18)
C14—O3—C17	119.1 (2)	C1—C2—H2	121.00
C1—N1—C7	105.29 (15)	C3—C2—H2	121.00
C6—N2—C7	106.36 (14)	C3—C4—H4	119.00
C6—N2—C18	123.58 (15)	C5—C4—H4	119.00
C7—N2—C18	129.87 (15)	C4—C5—H5	121.00
N1—C1—C2	130.85 (17)	C6—C5—H5	121.00
N1—C1—C6	109.99 (16)	O2—C9—H9A	110.00
C2—C1—C6	119.16 (17)	O2—C9—H9B	110.00
C1—C2—C3	118.69 (17)	C10—C9—H9A	110.00
C2—C3—C4	120.58 (18)	C10—C9—H9B	110.00
C2—C3—C8	118.27 (17)	H9A—C9—H9B	108.00
C4—C3—C8	121.14 (17)	C9—C10—H10A	109.00
C3—C4—C5	121.33 (18)	C9—C10—H10B	109.00
C4—C5—C6	117.23 (17)	C9—C10—H10C	109.00

N2—C6—C1	105.84 (15)	H10A—C10—H10B	109.00
N2—C6—C5	131.18 (17)	H10A—C10—H10C	110.00
C1—C6—C5	122.97 (17)	H10B—C10—H10C	109.00
N1—C7—N2	112.51 (15)	C11—C12—H12	119.00
N1—C7—C11	124.42 (16)	C13—C12—H12	119.00
N2—C7—C11	123.08 (16)	C12—C13—H13	120.00
O1—C8—O2	122.92 (19)	C14—C13—H13	120.00
O1—C8—C3	124.12 (19)	C14—C15—H15	120.00
O2—C8—C3	112.97 (17)	C16—C15—H15	120.00
O2—C9—C10	108.7 (3)	C11—C16—H16	119.00
C7—C11—C12	122.24 (16)	C15—C16—H16	119.00
C7—C11—C16	120.09 (17)	O3—C17—H17A	109.00
C12—C11—C16	117.65 (18)	O3—C17—H17B	109.00
C11—C12—C13	121.07 (18)	O3—C17—H17C	109.00
C12—C13—C14	120.4 (2)	H17A—C17—H17B	110.00
O3—C14—C13	115.3 (2)	H17A—C17—H17C	110.00
O3—C14—C15	124.73 (19)	H17B—C17—H17C	109.00
C13—C14—C15	119.9 (2)	N2—C18—H18A	109.00
C14—C15—C16	119.8 (2)	N2—C18—H18B	109.00
C11—C16—C15	121.2 (2)	C19—C18—H18A	109.00
N2—C18—C19	114.93 (15)	C19—C18—H18B	109.00
C18—C19—C20	123.82 (16)	H18A—C18—H18B	108.00
C18—C19—C24	117.67 (15)	C19—C20—H20	120.00
C20—C19—C24	118.50 (17)	C21—C20—H20	120.00
C19—C20—C21	120.57 (18)	C20—C21—H21	121.00
C20—C21—C22	118.64 (19)	C22—C21—H21	121.00
F1—C22—C21	118.57 (19)	C22—C23—H23	121.00
F1—C22—C23	118.8 (2)	C24—C23—H23	121.00
C21—C22—C23	122.6 (2)	C19—C24—H24	119.00
C22—C23—C24	118.1 (2)	C23—C24—H24	119.00
C9—O2—C8—O1	-0.7 (3)	C4—C3—C8—O1	175.9 (2)
C9—O2—C8—C3	179.00 (19)	C4—C3—C8—O2	-3.8 (3)
C8—O2—C9—C10	171.5 (2)	C3—C4—C5—C6	0.3 (3)
C17—O3—C14—C13	163.7 (3)	C4—C5—C6—N2	-179.81 (18)
C17—O3—C14—C15	-17.0 (4)	C4—C5—C6—C1	1.7 (3)
C7—N1—C1—C2	-179.0 (2)	N1—C7—C11—C12	-139.31 (19)
C7—N1—C1—C6	1.1 (2)	N1—C7—C11—C16	38.9 (3)
C1—N1—C7—N2	-0.5 (2)	N2—C7—C11—C12	41.0 (3)
C1—N1—C7—C11	179.72 (17)	N2—C7—C11—C16	-140.85 (19)
C7—N2—C6—C1	0.87 (19)	C7—C11—C12—C13	179.22 (18)
C7—N2—C6—C5	-177.82 (19)	C16—C11—C12—C13	1.0 (3)
C18—N2—C6—C1	176.28 (16)	C7—C11—C16—C15	-178.68 (19)
C18—N2—C6—C5	-2.4 (3)	C12—C11—C16—C15	-0.4 (3)
C6—N2—C7—N1	-0.2 (2)	C11—C12—C13—C14	-0.6 (3)
C6—N2—C7—C11	179.54 (16)	C12—C13—C14—O3	178.9 (2)
C18—N2—C7—N1	-175.24 (17)	C12—C13—C14—C15	-0.4 (3)
C18—N2—C7—C11	4.5 (3)	O3—C14—C15—C16	-178.3 (2)

C6—N2—C18—C19	85.6 (2)	C13—C14—C15—C16	0.9 (3)
C7—N2—C18—C19	-100.2 (2)	C14—C15—C16—C11	-0.5 (3)
N1—C1—C2—C3	-178.97 (19)	N2—C18—C19—C20	4.7 (3)
C6—C1—C2—C3	1.0 (3)	N2—C18—C19—C24	-176.44 (16)
N1—C1—C6—N2	-1.2 (2)	C18—C19—C20—C21	178.77 (18)
N1—C1—C6—C5	177.60 (17)	C24—C19—C20—C21	-0.1 (3)
C2—C1—C6—N2	178.81 (16)	C18—C19—C24—C23	-178.88 (19)
C2—C1—C6—C5	-2.4 (3)	C20—C19—C24—C23	0.0 (3)
C1—C2—C3—C4	0.9 (3)	C19—C20—C21—C22	0.2 (3)
C1—C2—C3—C8	179.53 (17)	C20—C21—C22—F1	179.9 (2)
C2—C3—C4—C5	-1.6 (3)	C20—C21—C22—C23	-0.3 (3)
C8—C3—C4—C5	179.83 (18)	F1—C22—C23—C24	-179.98 (19)
C2—C3—C8—O1	-2.7 (3)	C21—C22—C23—C24	0.3 (3)
C2—C3—C8—O2	177.62 (17)	C22—C23—C24—C19	-0.1 (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>
C17—H17C \cdots O1 ⁱ	0.96	2.43	3.356 (4)	163
C20—H20 \cdots O1 ⁱⁱ	0.93	2.45	3.324 (2)	156

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+1, -y, -z+1$.