ISSN 2414-3146

Received 28 October 2016 Accepted 31 October 2016

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

IUCrData

Keywords: crystal structure; benzoimidazole; methoxyphenyl; fluorobenzyl; C $-H\cdots$ O hydrogen bonds.

CCDC reference: 1513685

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

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

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The title benzoimidazole derivative, $C_{24}H_{21}FN_2O_3$, 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 $R_2^2(28)$ and $R_2^2(22)$ ring motifs. As a result of these hydrogen bonds, ribbons propagating along [010] are formed.



Structure description

Benzoimidazole-based compounds possess diverse biological activities such as anticancer, 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 benzoimidazole ring system. The fluorobenzyl and methoxyphenyl rings are inclined to one another by 78.9 (1)°. The benzoimidazole 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)° for torsion angle C15-C14-O3-C17. The mean plane of the ethyl carboxylate group (O1/O2/C8–C10) is inclined to the benzoimidazole ring by 4.53 (12)°.

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, °).	

$D - H \cdot \cdot \cdot A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - H \cdot \cdot \cdot A$
$\begin{array}{c} \text{C17}{-}\text{H17}\text{C}{\cdots}\text{O1}^{\text{i}}\\ \text{C20}{-}\text{H20}{\cdots}\text{O1}^{\text{ii}} \end{array}$	0.96	2.43	3.356 (4)	163
	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 det

Experimer	ntal d	letail	s.

Crystal data	
Chemical formula	$C_{24}H_{21}FN_2O_3$
M _r	404.43
Crystal system, space group	Monoclinic, $P2_1/n$
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)
$V(A^3)$	2049.7 (3)
Ζ	4
Radiation type	Cu Ka
$\mu \text{ (mm}^{-1})$	0.77
Crystal size (mm)	$0.29 \times 0.27 \times 0.24$
Data collection	
Diffractometer	Bruker X8 Proteum
Absorption correction	Multi-scan (SADABS; Bruker, 2013)
T_{\min}, T_{\max}	0.808, 0.837
No. of measured, independent and observed $[I > 2\sigma(I)]$ reflections	12703, 3318, 2930
R _{int}	0.053
$(\sin \theta / \lambda)_{\max} (\mathring{A}^{-1})$	0.584
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.062, 0.182, 1.05
No. of reflections	3318
No. of parameters	274
H-atom treatment	H-atom parameters constrained
$\Delta \rho_{\rm max}, \Delta \rho_{\rm min} \ ({\rm e} \ {\rm \AA}^{-3})$	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.

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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-5carboxylate

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

Crystal data

C₂₄H₂₁FN₂O₃ $M_r = 404.43$ Monoclinic, P2₁/n Hall symbol: -P 2yn a = 13.5156 (10) Å b = 9.5906 (8) Å c = 16.1315 (13) Å $\beta = 101.409$ (3)° V = 2049.7 (3) Å³ Z = 4

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)

Refinement

Refinement on F^2 Least-squares matrix: full $R[F^2 > 2\sigma(F^2)] = 0.062$ $wR(F^2) = 0.182$ S = 1.053318 reflections 274 parameters 0 restraints Primary atom site location: structure-invariant direct methods Secondary atom site location: difference Fourier map F(000) = 848 $D_x = 1.311 \text{ Mg m}^{-3}$ Cu K\alpha radiation, $\lambda = 1.54178 \text{ Å}$ Cell parameters from 2930 reflections $\theta = 4.8-64.2^{\circ}$ $\mu = 0.77 \text{ mm}^{-1}$ T = 296 KBlock, colourless $0.29 \times 0.27 \times 0.24 \text{ mm}$

 $T_{\min} = 0.808, T_{\max} = 0.837$ 12703 measured reflections
3318 independent reflections
2930 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.053$ $\theta_{\text{max}} = 64.2^{\circ}, \theta_{\text{min}} = 4.8^{\circ}$ $h = -15 \rightarrow 15$ $k = -9 \rightarrow 10$ $l = -17 \rightarrow 18$

Hydrogen site location: inferred from neighbouring sites H-atom parameters constrained $w = 1/[\sigma^2(F_o^2) + (0.1193P)^2 + 0.3084P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{max} < 0.001$ $\Delta\rho_{max} = 0.21$ e Å⁻³ $\Delta\rho_{min} = -0.22$ e Å⁻³ Extinction correction: SHELXL97 (Sheldrick, 2008), FC*=KFC[1+0.001XFC^2\Lambda^3/SIN(2\Theta)]^{-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 $F^2 > 2sigma(F^2)$ 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.

 $U_{iso} * / U_{eq}$ х Zv F1 0.0973 (6) 1.07749 (10) -0.11559(17)0.77837(11) **O**1 0.0797 (6) 0.26807(12) -0.0335(2)0.51786 (10) O2 0.31003 (11) -0.14020(17)0.64310(10) 0.0721 (6) O3 0.0922 (7) 0.94650 (14) 0.72073 (18) 0.50713 (14) 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) 0.0527(6)0.1219(2)0.55256(12)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) 0.84310 (13) C19 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)0.82863 (14) C23 0.99693 (16) 0.0737(3)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 -0.050900.46300 0.72870 0.0660* H5 0.61270 0.07070 0.76760 0.0640* H9A 0.21030 -0.264000.56990 0.1100* H9B 0.16000 -0.159500.62440 0.1100*

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters $(Å^2)$

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 (\mathring{A}^2)

	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)

data reports

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)	С2—Н2	0.9300
N1—C7	1.314 (2)	C4—H4	0.9300
N2—C6	1.375 (2)	С5—Н5	0.9300
N2—C7	1.390 (2)	С9—Н9А	0.9700
N2-C18	1.452 (2)	С9—Н9В	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
С8—О2—С9	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)	С6—С5—Н5	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)	С10—С9—Н9А	110.00
C2—C3—C4	120.58 (18)	С10—С9—Н9В	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	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
01-C8-02	122.92 (19)	C14—C13—H13	120.00
01 - C8 - C3	124 12 (19)	C14—C15—H15	120.00
$0^{2}-0^{8}-0^{3}$	112.97 (17)	C16—C15—H15	120.00
02 - 00 - 010	108.7(3)	$C_{11} - C_{16} - H_{16}$	119.00
C7-C11-C12	122 24 (16)	C_{15} C_{16} H_{16}	119.00
C7 - C11 - C12	122.24(10) 120.09(17)	$03 - C_{17} - H_{17A}$	109.00
C_1^2 C_1^1 C_1^6	120.09(17) 117.65(18)	$O_3 = C_{17} = H_{17R}$	109.00
C_{12} C_{12} C_{13} C_{13}	117.03(18) 121.07(18)	03 - C17 - H17C	109.00
$C_{12} = C_{12} = C_{13}$	121.07(10) 120.4(2)	03-017-017	109.00
C12 - C13 - C14	120.4(2)	HI/A - CI/-HI/B	110.00
03 - C14 - C13	115.5(2)	HI/A = CI/=HI/C	110.00
03-014-015	124.73 (19)	HI/B—CI/—HI/C	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)	C_{16} C_{11} C_{12} C_{13}	10(3)
$C_{18} N_{2} C_{6} C_{1}$	176 28 (16)	C7-C11-C16-C15	-17868(19)
C18 N2 C6 C1	-2.4(3)	C_{12} $-C_{11}$ $-C_{16}$ $-C_{15}$	-0.4(3)
$C6_N2_C7_N1$	-0.2(2)	C11 - C12 - C13 - C14	-0.6(3)
$C_{0} = 12 = C_{1} = 101$ $C_{0} = 102 = C_{1} = 101$	17954(16)	C12 - C13 - C14 - O3	$178 \ 0 \ (2)$
C18 N2 C7 N1	-175 24 (10)	$C_{12} = C_{13} = C_{14} = C_{15}$	-0.1(2)
$C_{10} = N_2 = C_7 = N_1$	1/3.24(1/)	03 C14 C15 C16	-1792(2)
$U_{10} - W_2 - U_1 - U_{11}$	4.5 (5)	03 - 014 - 013 - 010	1/0.3 (2)

C6-N2-C18-C19	85.6 (2)	C_{13} C_{14} C_{15} C_{16}	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, °)

D—H···A	D—H	H···A	D···A	D—H··· A
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.