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Diethyl 3,3′-[(3-fluorophenyl)methylene]bis(1*H*-indole-2-carboxylate)

Hong Jiang,[a] Yu-Long Li,[a] Jin Zhou,[a,b] Hong-Shun Sun,[a]* Qing-Yu Zhang,[a] Xing-Hao Shi,[a] Zhi-Yuan Zhang[a] and Tian Ling[a]

[a]Targeted MRI Contrast Agents Laboratory of Jiangsu Province, Nanjing Polytechnic Institute, Nanjing 210048, People's Republic of China, and [b]College of Chemistry and Molecular Engineering, Nanjing Tech University, Nanjing 211816, People's Republic of China. *Correspondence e-mail: njutshs@126.com

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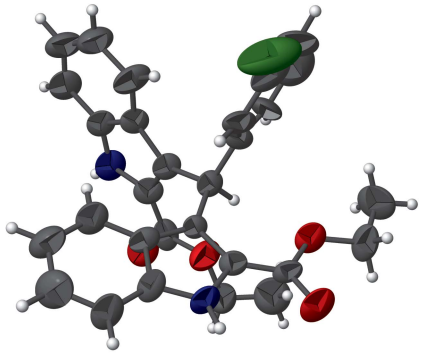
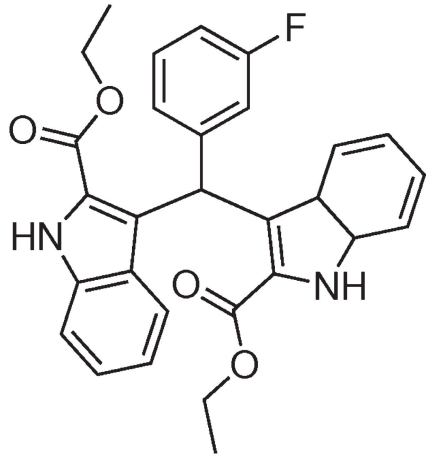
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{29}H_{25}FN_2O_4$, the mean planes of the indole ring systems are approximately perpendicular to one another [dihedral angle = 88.3 (4)°]. The benzene ring is twisted with respect to the indole ring systems by 49.8 (5) and 77.6 (3)°. In the crystal, pairs of N—H···O hydrogen bonds link the molecules into the inversion dimers which are further linked into supramolecular chains propagating along the [110] direction.

3D view



Chemical scheme



Structure description

There are abundant bis(indolyl)methane derivatives in various terrestrial and marine natural resources (Sundberg, 1996). As part of our ongoing studies of bis(indoyl)methane compounds, we now report the synthesis and crystal structure of the title compound.

The molecular structure of the title compound is shown in Fig. 1. The indole ring systems are nearly perpendicular to one another [dihedral angle = 88.3 (4)°] while the benzene ring (C2–C7) is twisted with respect to the N1/C8–C15 and N2/C19–C26 indole ring systems with dihedral angles of 49.8 (5) and 77.6 (3)°, respectively. The carboxyl groups are approximately co-planar with their attached indole ring systems, the dihedral angles between the carboxyl groups and the mean planes of the N1/C8–C15 and N2/C19–C26 indole ring systems being 6.2 (5) and 6.4 (4)°, respectively.

In the crystal, pairwise N1—H1*A*···O1^{i} and N2—H2*A*···O4^{ii} hydrogen bonds both generate $R_2^2(8)$ loops; together these lead to [110] chains of molecules. A weak C11—H11*A*···O4^{iii} interaction also occurs, which links the chains into (001) sheets (Table 1 and Fig. 2).

Several similar structures have been reported previously, *viz*. diethyl 3,3′-(phenylmethylene)bis(1*H*-indole-2-carboxylate) (Sun *et al.*, 2012), dimethyl 3,3′-[(3-fluoro-

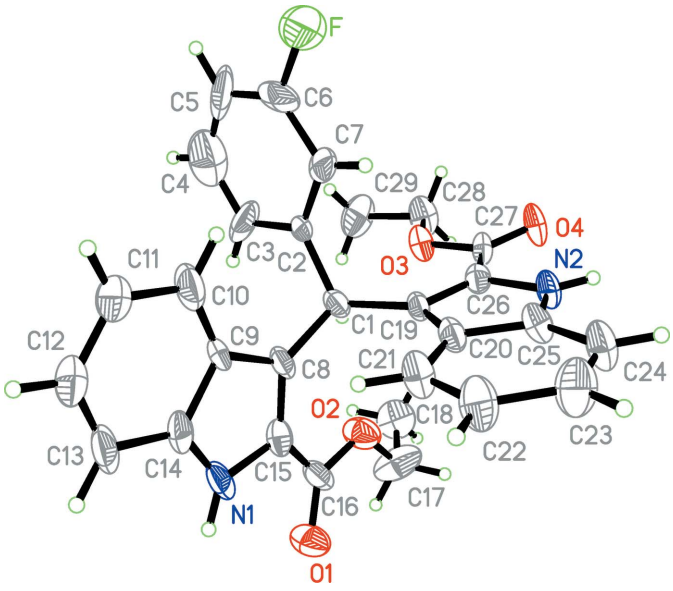


Figure 1
The molecular structure of the title molecule with displacement ellipsoids drawn at the 30% probability level.

phenyl)methylene]bis(1*H*-indole-2-carboxylate) (Lu *et al.*, 2014), dimethyl 3,3′-[(4-fluorophenyl)methylene]bis(1*H*-indole-2-carboxylate) (Sun *et al.*, 2015) and dimethyl 3,3′-[(2-fluorophenyl)methylene]bis(1*H*-indole-2-carboxylate) (Lu *et al.*, 2017). In these structures, the indole ring systems are also nearly perpendicular to one another, making dihedral angles of 82.0 (5), 87.8 (5), 84.0 (5) and 86.0 (5)°, respectively.

Synthesis and crystallization

Ethyl indole-2-carboxylate (1.88 g, 10 mmol) was dissolved in 20 ml of ethanol and 3-fluorobenzaldehyde (0.62 g, 5 mmol) and concentrated HCl (0.5 ml) was added. The mixture was heated to reflux temperature for 2 h. After cooling, the white product was filtered off and washed thoroughly with ethanol (yield = 92%). Single crystals of the title compound suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution.

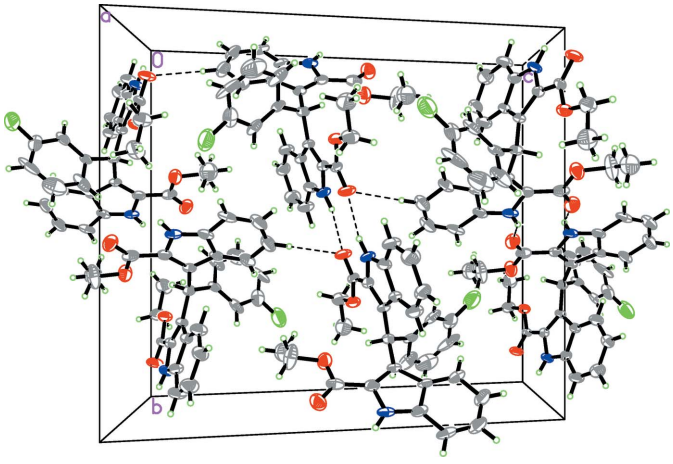


Figure 2
A packing diagram of the title compound. Hydrogen bonds are shown as dashed lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1^{i}	0.86	2.16	2.918 (11)	147
N2—H2A···O4^{ii}	0.86	2.08	2.904 (9)	159
C11—H11A···O4^{iii}	0.93	2.58	3.498 (13)	171

Symmetry codes: (i) $-x, -y, -z+1$; (ii) $-x+1, -y+1, -z+1$; (iii) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{29}H_{25}FN_2O_4$
M_r	484.51
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	293
a, b, c (Å)	8.9960 (18), 15.921 (3), 18.297 (4)
β (°)	102.59 (3)
V (Å^3)	2557.6 (9)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.20 × 0.20 × 0.10
Data collection	
Diffractometer	Enraf–Nonius CAD-4
Absorption correction	ψ scan (North *et al.*, 1968)
T_{min}, T_{max}	0.982, 0.991
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5000, 4685, 1424
R_{int}	0.131
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.603
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.143, 0.306, 1.30
No. of reflections	4685
No. of parameters	319
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.56, −0.72

Computer programs: *CAD-4 EXPRESS* (Enraf–Nonius, 1994), *XCAD4* (Harms & Wocadlo, 1995) and *SHELXTL* (Sheldrick, 2008).

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2020). **5**, x200912 [https://doi.org/10.1107/S2414314620009128]

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Crystal data

$C_{29}H_{25}FN_2O_4$
M_r = 484.51
Monoclinic, $P2_1/n$
a = 8.9960 (18) Å
b = 15.921 (3) Å
c = 18.297 (4) Å
β = 102.59 (3)°
V = 2557.6 (9) Å^3
Z = 4
$F(000)$ = 1016
D_x = 1.258 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 25 reflections
θ = 9–12°
μ = 0.09 mm^{-1}
T = 293 K
Block, colorless
0.20 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.982, T_{max} = 0.991
5000 measured reflections
4685 independent reflections
1424 reflections with $I > 2\sigma(I)$
R_{int} = 0.131
θ_{max} = 25.4°, θ_{min} = 1.7°
h = 0→10
k = 0→19
l = −22→21
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.143
$wR(F^2)$ = 0.306
S = 1.30
4685 reflections
319 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
$w = 1/[\sigma^2(F_o^2) + (0.060P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.009
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.71 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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.
H atoms were positioned geometrically with N—H = 0.86 Å and C—H = 0.93–0.98 Å, and constrained to ride on their parent atoms. The constraint $U_{iso}(H) = 1.2U_{eq}(C,N)$ or $1.5U_{eq}$(methyl C) was applied in all cases.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
F	0.5574 (10)	0.2828 (5)	0.1783 (4)	0.154 (4)
O1	0.1733 (8)	0.0523 (4)	0.5601 (4)	0.080 (2)
N1	0.0972 (9)	0.0284 (4)	0.4084 (5)	0.063 (2)
H1A	0.0468	−0.0028	0.4327	0.076*
C1	0.3860 (9)	0.1906 (5)	0.3962 (5)	0.045 (2)
H1B	0.4561	0.1763	0.4434	0.054*
N2	0.3321 (8)	0.4124 (4)	0.4463 (4)	0.054 (2)
H2A	0.3634	0.4597	0.4668	0.064*
O2	0.3615 (8)	0.1390 (4)	0.5478 (4)	0.078 (2)
C2	0.4782 (11)	0.1845 (6)	0.3395 (6)	0.049 (3)
O3	0.6571 (7)	0.2781 (3)	0.4797 (3)	0.0609 (19)
C3	0.5727 (12)	0.1140 (8)	0.3428 (7)	0.094 (5)
H3A	0.5770	0.0753	0.3812	0.112*
O4	0.6412 (7)	0.4138 (4)	0.5044 (4)	0.071 (2)
C4	0.659 (2)	0.1009 (11)	0.2907 (12)	0.143 (7)
H4A	0.7197	0.0531	0.2945	0.172*
C5	0.6584 (19)	0.1558 (11)	0.2334 (11)	0.129 (7)
H5A	0.7151	0.1471	0.1972	0.155*
C6	0.5694 (16)	0.2231 (10)	0.2335 (7)	0.092 (4)
C7	0.4733 (12)	0.2417 (7)	0.2840 (6)	0.071 (3)
H7A	0.4121	0.2893	0.2792	0.086*
C8	0.2671 (10)	0.1236 (5)	0.3855 (6)	0.050 (3)
C9	0.1838 (10)	0.0882 (5)	0.3150 (6)	0.051 (3)
C10	0.1875 (12)	0.1021 (6)	0.2409 (7)	0.080 (4)
H10A	0.2524	0.1420	0.2276	0.096*
C11	0.0911 (12)	0.0547 (7)	0.1867 (6)	0.082 (4)
H11A	0.0929	0.0626	0.1366	0.099*
C12	−0.0061 (14)	−0.0033 (7)	0.2053 (7)	0.088 (4)
H12A	−0.0678	−0.0341	0.1673	0.105*
C13	−0.0162 (12)	−0.0175 (6)	0.2762 (7)	0.077 (3)
H13A	−0.0844	−0.0565	0.2878	0.092*
C14	0.0816 (11)	0.0295 (6)	0.3329 (7)	0.058 (3)
C15	0.2065 (11)	0.0855 (6)	0.4391 (6)	0.057 (3)
C16	0.2487 (12)	0.0887 (6)	0.5223 (7)	0.061 (3)

C17	0.4070 (12)	0.1489 (9)	0.6278 (6)	0.108 (5)
H17A	0.3662	0.2010	0.6427	0.129*
H17B	0.3673	0.1029	0.6525	0.129*
C18	0.5630 (13)	0.1500 (7)	0.6483 (7)	0.112
H18A	0.5940	0.1565	0.7016	0.168*
H18B	0.6015	0.1960	0.6241	0.168*
H18C	0.6027	0.0982	0.6337	0.168*
C19	0.3282 (9)	0.2778 (5)	0.4087 (5)	0.039 (2)
C20	0.1817 (11)	0.3129 (5)	0.3856 (5)	0.049 (3)
C21	0.0406 (12)	0.2819 (6)	0.3459 (6)	0.069 (3)
H21A	0.0315	0.2268	0.3286	0.082*
C22	−0.0847 (13)	0.3351 (7)	0.3330 (6)	0.077 (4)
H22A	−0.1789	0.3152	0.3073	0.092*
C23	−0.0710 (13)	0.4196 (7)	0.3585 (6)	0.089 (4)
H23A	−0.1560	0.4544	0.3490	0.106*
C24	0.0652 (12)	0.4502 (6)	0.3968 (6)	0.071 (3)
H24A	0.0749	0.5056	0.4131	0.085*
C25	0.1893 (11)	0.3958 (5)	0.4105 (5)	0.054 (3)
C26	0.4231 (11)	0.3414 (5)	0.4456 (5)	0.044 (2)
C27	0.5740 (11)	0.3489 (5)	0.4795 (5)	0.045 (2)
C28	0.8156 (10)	0.2802 (6)	0.5124 (6)	0.075 (3)
H28A	0.8324	0.2942	0.5651	0.089*
H28B	0.8662	0.3218	0.4877	0.089*
C29	0.8750 (12)	0.1962 (7)	0.5028 (6)	0.101 (4)
H29A	0.9824	0.1948	0.5241	0.152*
H29B	0.8573	0.1830	0.4504	0.152*
H29C	0.8242	0.1557	0.5276	0.152*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F	0.256 (10)	0.129 (7)	0.088 (6)	−0.081 (7)	0.063 (6)	−0.033 (5)
O1	0.085 (6)	0.085 (5)	0.073 (6)	−0.020 (4)	0.022 (4)	0.013 (4)
N1	0.076 (6)	0.026 (4)	0.088 (7)	−0.012 (4)	0.016 (6)	−0.001 (5)
C1	0.050 (6)	0.033 (5)	0.053 (7)	−0.012 (5)	0.011 (5)	0.000 (5)
N2	0.058 (5)	0.031 (4)	0.065 (6)	−0.009 (4)	0.001 (5)	−0.015 (4)
O2	0.081 (5)	0.091 (6)	0.060 (5)	−0.032 (5)	0.014 (4)	−0.005 (4)
C2	0.057 (7)	0.035 (6)	0.065 (8)	−0.025 (5)	0.033 (6)	−0.021 (5)
O3	0.068 (5)	0.036 (4)	0.072 (5)	0.002 (4)	0.001 (4)	−0.004 (3)
C3	0.068 (8)	0.109 (11)	0.117 (12)	−0.005 (8)	0.049 (8)	−0.068 (9)
O4	0.079 (5)	0.030 (4)	0.093 (5)	−0.004 (4)	−0.008 (4)	−0.016 (4)
C4	0.132 (15)	0.105 (14)	0.18 (2)	−0.017 (12)	0.016 (15)	−0.038 (13)
C5	0.132 (14)	0.101 (13)	0.169 (19)	−0.033 (12)	0.065 (14)	−0.106 (13)
C6	0.113 (11)	0.097 (11)	0.066 (10)	−0.081 (9)	0.022 (9)	−0.013 (9)
C7	0.079 (8)	0.067 (8)	0.077 (9)	−0.039 (7)	0.036 (7)	−0.046 (7)
C8	0.062 (7)	0.025 (5)	0.061 (7)	−0.011 (5)	0.013 (6)	−0.002 (5)
C9	0.063 (7)	0.025 (5)	0.069 (8)	−0.017 (5)	0.023 (6)	−0.012 (6)
C10	0.104 (9)	0.053 (7)	0.077 (9)	−0.029 (6)	0.009 (8)	−0.024 (7)

C11	0.097 (9)	0.081 (8)	0.070 (9)	−0.023 (7)	0.021 (7)	−0.029 (7)
C12	0.105 (10)	0.074 (9)	0.084 (10)	−0.019 (8)	0.023 (9)	−0.040 (8)
C13	0.084 (8)	0.034 (6)	0.112 (10)	−0.010 (6)	0.019 (8)	−0.028 (7)
C14	0.063 (7)	0.032 (6)	0.076 (9)	0.006 (5)	0.006 (7)	−0.015 (6)
C15	0.069 (7)	0.031 (6)	0.067 (8)	0.007 (5)	0.010 (7)	−0.003 (6)
C16	0.053 (7)	0.039 (6)	0.094 (10)	−0.010 (6)	0.022 (7)	0.006 (6)
C17	0.062 (8)	0.200 (14)	0.058 (9)	−0.006 (8)	0.008 (7)	−0.030 (9)
C18	0.112	0.112	0.112	0.000	0.024	0.000
C19	0.041 (6)	0.026 (5)	0.049 (6)	−0.005 (4)	0.010 (5)	−0.006 (4)
C20	0.065 (7)	0.032 (5)	0.047 (6)	−0.009 (5)	0.008 (6)	−0.004 (5)
C21	0.072 (8)	0.042 (6)	0.085 (9)	−0.001 (6)	0.003 (7)	−0.010 (6)
C22	0.089 (9)	0.061 (8)	0.070 (8)	−0.002 (7)	−0.008 (7)	−0.015 (6)
C23	0.086 (9)	0.072 (8)	0.098 (10)	0.028 (7)	−0.002 (8)	−0.001 (8)
C24	0.068 (8)	0.039 (6)	0.097 (9)	−0.002 (6)	−0.003 (7)	−0.013 (6)
C25	0.054 (7)	0.036 (6)	0.063 (7)	−0.001 (5)	−0.007 (6)	0.004 (5)
C26	0.053 (6)	0.036 (5)	0.044 (6)	0.003 (5)	0.009 (5)	−0.001 (5)
C27	0.060 (7)	0.030 (5)	0.042 (6)	0.006 (5)	0.001 (5)	−0.008 (5)
C28	0.053 (7)	0.056 (7)	0.100 (9)	0.015 (6)	−0.016 (7)	0.001 (6)
C29	0.097 (9)	0.099 (9)	0.104 (10)	0.053 (8)	0.012 (8)	−0.007 (8)

Geometric parameters (Å, º)

F—C6	1.374 (13)	C11—C12	1.365 (13)
O1—C16	1.216 (10)	C11—H11A	0.9300
N1—C14	1.356 (11)	C12—C13	1.339 (13)
N1—C15	1.367 (10)	C12—H12A	0.9300
N1—H1A	0.8600	C13—C14	1.418 (12)
C1—C2	1.464 (11)	C13—H13A	0.9300
C1—C8	1.492 (10)	C15—C16	1.488 (13)
C1—C19	1.517 (10)	C17—C18	1.371 (12)
C1—H1B	0.9800	C17—H17A	0.9700
N2—C25	1.335 (10)	C17—H17B	0.9700
N2—C26	1.398 (9)	C18—H18A	0.9600
N2—H2A	0.8600	C18—H18B	0.9600
O2—C16	1.297 (10)	C18—H18C	0.9600
O2—C17	1.440 (11)	C19—C26	1.399 (10)
C2—C7	1.359 (13)	C19—C20	1.409 (11)
C2—C3	1.401 (13)	C20—C25	1.394 (11)
O3—C27	1.351 (9)	C20—C21	1.407 (11)
O3—C28	1.421 (9)	C21—C22	1.389 (12)
C3—C4	1.370 (18)	C21—H21A	0.9300
C3—H3A	0.9300	C22—C23	1.420 (12)
O4—C27	1.234 (9)	C22—H22A	0.9300
C4—C5	1.363 (19)	C23—C24	1.361 (12)
C4—H4A	0.9300	C23—H23A	0.9300
C5—C6	1.339 (18)	C24—C25	1.392 (11)
C5—H5A	0.9300	C24—H24A	0.9300
C6—C7	1.426 (15)	C26—C27	1.370 (11)

C7—H7A	0.9300	C28—C29	1.465 (11)
C8—C15	1.364 (11)	C28—H28A	0.9700
C8—C9	1.457 (12)	C28—H28B	0.9700
C9—C10	1.382 (12)	C29—H29A	0.9600
C9—C14	1.400 (11)	C29—H29B	0.9600
C10—C11	1.389 (12)	C29—H29C	0.9600
C10—H10A	0.9300		

C14—N1—C15	108.4 (9)	C8—C15—C16	131.9 (10)
C14—N1—H1A	125.8	O1—C16—O2	125.4 (11)
C15—N1—H1A	125.8	O1—C16—C15	121.1 (10)
C2—C1—C8	111.1 (7)	O2—C16—C15	113.2 (10)
C2—C1—C19	115.7 (7)	C18—C17—O2	109.1 (10)
C8—C1—C19	114.4 (7)	C18—C17—H17A	109.9
C2—C1—H1B	104.7	O2—C17—H17A	109.9
C8—C1—H1B	104.7	C18—C17—H17B	109.9
C19—C1—H1B	104.7	O2—C17—H17B	109.9
C25—N2—C26	109.7 (7)	H17A—C17—H17B	108.3
C25—N2—H2A	125.1	C17—C18—H18A	109.5
C26—N2—H2A	125.1	C17—C18—H18B	109.5
C16—O2—C17	117.4 (9)	H18A—C18—H18B	109.5
C7—C2—C3	119.2 (11)	C17—C18—H18C	109.5
C7—C2—C1	123.7 (10)	H18A—C18—H18C	109.5
C3—C2—C1	117.1 (10)	H18B—C18—H18C	109.5
C27—O3—C28	119.0 (7)	C26—C19—C20	106.9 (7)
C4—C3—C2	121.6 (15)	C26—C19—C1	122.8 (8)
C4—C3—H3A	119.2	C20—C19—C1	130.2 (7)
C2—C3—H3A	119.2	C25—C20—C21	118.4 (9)
C3—C4—C5	122.0 (19)	C25—C20—C19	107.5 (8)
C3—C4—H4A	119.0	C21—C20—C19	134.1 (8)
C5—C4—H4A	119.0	C22—C21—C20	118.8 (9)
C6—C5—C4	114.4 (18)	C22—C21—H21A	120.6
C6—C5—H5A	122.8	C20—C21—H21A	120.6
C4—C5—H5A	122.8	C21—C22—C23	120.8 (10)
C5—C6—F	120.2 (17)	C21—C22—H22A	119.6
C5—C6—C7	127.9 (14)	C23—C22—H22A	119.6
F—C6—C7	111.8 (15)	C24—C23—C22	120.8 (10)
C2—C7—C6	114.8 (11)	C24—C23—H23A	119.6
C2—C7—H7A	122.6	C22—C23—H23A	119.6
C6—C7—H7A	122.6	C23—C24—C25	117.8 (9)
C15—C8—C9	104.8 (8)	C23—C24—H24A	121.1
C15—C8—C1	127.7 (9)	C25—C24—H24A	121.1
C9—C8—C1	127.4 (9)	N2—C25—C24	127.8 (9)
C10—C9—C14	119.6 (10)	N2—C25—C20	108.8 (8)
C10—C9—C8	133.6 (9)	C24—C25—C20	123.4 (9)
C14—C9—C8	106.8 (9)	C27—C26—N2	116.7 (8)
C11—C10—C9	117.9 (10)	C27—C26—C19	136.2 (8)
C11—C10—H10A	121.0	N2—C26—C19	107.1 (7)

C9—C10—H10A	121.0	O4—C27—O3	118.1 (8)
C12—C11—C10	121.6 (11)	O4—C27—C26	126.7 (8)
C12—C11—H11A	119.2	O3—C27—C26	114.9 (8)
C10—C11—H11A	119.2	O3—C28—C29	106.7 (8)
C13—C12—C11	122.5 (12)	O3—C28—H28A	110.4
C13—C12—H12A	118.7	C29—C28—H28A	110.4
C11—C12—H12A	118.7	O3—C28—H28B	110.4
C12—C13—C14	117.2 (11)	C29—C28—H28B	110.4
C12—C13—H13A	121.4	H28A—C28—H28B	108.6
C14—C13—H13A	121.4	C28—C29—H29A	109.5
N1—C14—C9	108.6 (9)	C28—C29—H29B	109.5
N1—C14—C13	130.4 (11)	H29A—C29—H29B	109.5
C9—C14—C13	121.0 (11)	C28—C29—H29C	109.5
N1—C15—C8	111.4 (9)	H29A—C29—H29C	109.5
N1—C15—C16	116.3 (10)	H29B—C29—H29C	109.5

C8—C1—C2—C7	110.8 (9)	C17—O2—C16—O1	3.8 (15)
C19—C1—C2—C7	−21.8 (13)	C17—O2—C16—C15	177.6 (9)
C8—C1—C2—C3	−67.4 (11)	N1—C15—C16—O1	−11.3 (14)
C19—C1—C2—C3	159.9 (8)	C8—C15—C16—O1	176.3 (10)
C7—C2—C3—C4	−0.8 (16)	N1—C15—C16—O2	174.6 (8)
C1—C2—C3—C4	177.5 (11)	C8—C15—C16—O2	2.1 (15)
C2—C3—C4—C5	1 (2)	C16—O2—C17—C18	138.6 (11)
C3—C4—C5—C6	1 (2)	C2—C1—C19—C26	−72.7 (11)
C4—C5—C6—F	−179.3 (12)	C8—C1—C19—C26	156.2 (8)
C4—C5—C6—C7	−3 (2)	C2—C1—C19—C20	104.3 (11)
C3—C2—C7—C6	−0.4 (13)	C8—C1—C19—C20	−26.8 (14)
C1—C2—C7—C6	−178.6 (8)	C26—C19—C20—C25	−1.7 (10)
C5—C6—C7—C2	2.2 (17)	C1—C19—C20—C25	−179.0 (9)
F—C6—C7—C2	179.2 (8)	C26—C19—C20—C21	179.0 (10)
C2—C1—C8—C15	149.4 (10)	C1—C19—C20—C21	1.6 (18)
C19—C1—C8—C15	−77.3 (12)	C25—C20—C21—C22	0.2 (15)
C2—C1—C8—C9	−34.5 (13)	C19—C20—C21—C22	179.5 (10)
C19—C1—C8—C9	98.8 (11)	C20—C21—C22—C23	0.8 (16)
C15—C8—C9—C10	177.8 (11)	C21—C22—C23—C24	−0.5 (18)
C1—C8—C9—C10	1.0 (17)	C22—C23—C24—C25	−0.6 (17)
C15—C8—C9—C14	−1.5 (10)	C26—N2—C25—C24	−177.8 (10)
C1—C8—C9—C14	−178.2 (8)	C26—N2—C25—C20	0.5 (11)
C14—C9—C10—C11	−1.9 (15)	C23—C24—C25—N2	179.7 (10)
C8—C9—C10—C11	178.9 (10)	C23—C24—C25—C20	1.7 (16)
C9—C10—C11—C12	0.9 (16)	C21—C20—C25—N2	−179.8 (8)
C10—C11—C12—C13	0.7 (19)	C19—C20—C25—N2	0.7 (11)
C11—C12—C13—C14	−1.2 (18)	C21—C20—C25—C24	−1.4 (15)
C15—N1—C14—C9	0.3 (10)	C19—C20—C25—C24	179.1 (9)
C15—N1—C14—C13	−179.8 (9)	C25—N2—C26—C27	179.2 (8)
C10—C9—C14—N1	−178.7 (9)	C25—N2—C26—C19	−1.5 (10)
C8—C9—C14—N1	0.7 (10)	C20—C19—C26—C27	−179.0 (11)
C10—C9—C14—C13	1.4 (14)	C1—C19—C26—C27	−1.4 (16)

C8—C9—C14—C13	−179.2 (8)	C20—C19—C26—N2	1.9 (10)
C12—C13—C14—N1	−179.8 (10)	C1—C19—C26—N2	179.5 (8)
C12—C13—C14—C9	0.1 (15)	C28—O3—C27—O4	3.8 (13)
C14—N1—C15—C8	−1.3 (11)	C28—O3—C27—C26	178.8 (8)
C14—N1—C15—C16	−175.3 (8)	N2—C26—C27—O4	−7.4 (14)
C9—C8—C15—N1	1.7 (10)	C19—C26—C27—O4	173.6 (10)
C1—C8—C15—N1	178.5 (8)	N2—C26—C27—O3	178.1 (7)
C9—C8—C15—C16	174.4 (9)	C19—C26—C27—O3	−1.0 (16)
C1—C8—C15—C16	−8.8 (16)	C27—O3—C28—C29	−178.8 (8)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O1^{i}	0.86	2.16	2.918 (11)	147
N2—H2*A*···O4^{ii}	0.86	2.08	2.904 (9)	159
C11—H11*A*···O4^{iii}	0.93	2.58	3.498 (13)	171

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