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5-Fluoro-1-(prop-2-en-1-yl)-2,3-dihydro-1*H*-indole-2,3-dione

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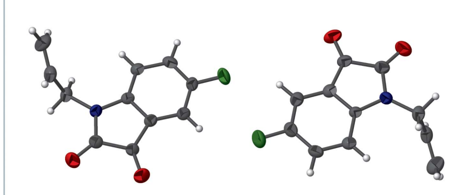
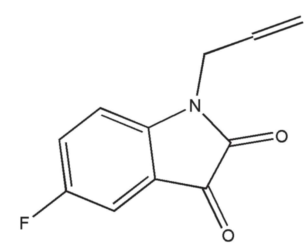
The asymmetric unit of the title compound, $C_{11}H_8FNO_2$, consists of two independent molecules having different conformations and associated through pairwise C—H···F hydrogen bonds. These units form 'stairstep' stacks along the *b*-axis direction *via* π–π stacking interactions between dihydroindole moieties, with interplanar spacings of 3.578 (3) and 3.627 (3) Å. The stacks are tied together by weak C—H···O hydrogen bonds.

3D view



Chemical scheme



Structure description

Isatin (1*H*-indole-2,3- dione) derivatives are synthetically versatile substrates, which can be used for the synthesis of a large variety of heterocyclic compounds and as raw material for drug synthesis. Compounds containing an isatin moiety are most widely used as anti-Parkinsonian (Knölker & Reddy, 2002), antifungal (Granik *et al.*, 1978) and anticancer agents (Marko *et al.*, 2001). Additionally, isatin derivatives find applications in chemistry of transition metal catalysts for uniform polymerization and in luminescence chemistry (Grandberg *et al.*, 1968). It has been shown that isatins exhibit antitumor activity due to the formation of stable complexes with DNA (Aravinda *et al.*, 2009). For the biological activity of isatin derivatives, see: Ramachandran (2011); Smitha *et al.* (2008).

As a continuation of our research devoted to the synthesis of isatin derivatives (Qachchachi *et al.*, 2014), we report here the synthesis and structure of 1-allyl-5-fluoroindoline-2,3-dione. The asymmetric unit consists of two independent molecules forming pseudo-centrosymmetric dimers associated through pairwise C5—H5···F2 and C16—H16···F1 hydrogen bonds (Table 1 and Fig. 1). These units form 'stairstep' stacks parallel

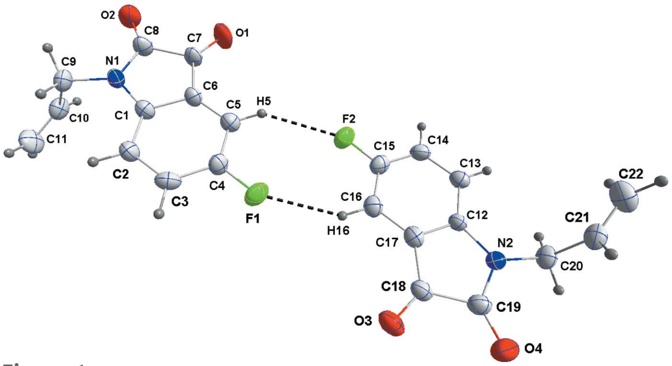


Figure 1
The asymmetric unit of the title compound, showing the atom-labeling scheme and 50% probability displacement ellipsoids. The C—H⋯F hydrogen bonds are shown as dotted lines.

to the *b* axis *via* π–π stacking interactions in which the N1,C1,C6–C8 ring associates with the C1–C6 ring of the corresponding molecule at x, $1 + y$, z while the C1–C6 ring associates with the N1,C1,C6–C8 ring of the corresponding molecule at x, $-1 + y$, z (Fig. 2). In both instances, the interplanar spacing is 3.578 (3) Å and the dihedral angle between the planes is 1.5 (2)°. Concurrently, the other half of the asymmetric unit forms analogous stacking interactions with its counterparts generated by the same symmetry operations with the interplanar spacing being 3.627 (3) Å and the dihedral angle 2.0 (2)°. Fig. 3 shows the packing of the complete unit cell. For the structure of 1-octylindoline-2,3-dione, see: Qachchachi *et al.* (2013).

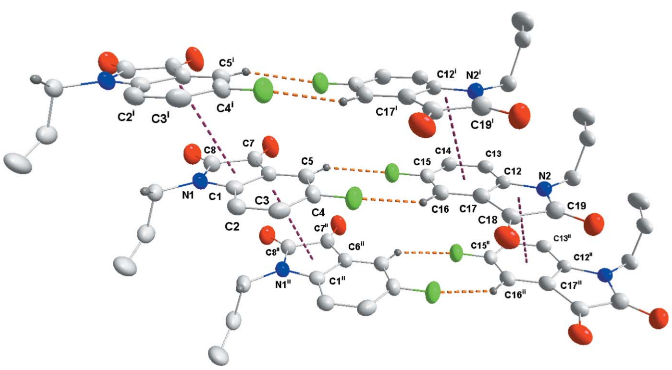


Figure 2
Detail of the π–π stacking in the crystal packing of the title compound (purple dotted lines). [Symmetry codes: (i) x, $1 + y$, z; (ii) x, $-1 + y$, z.]

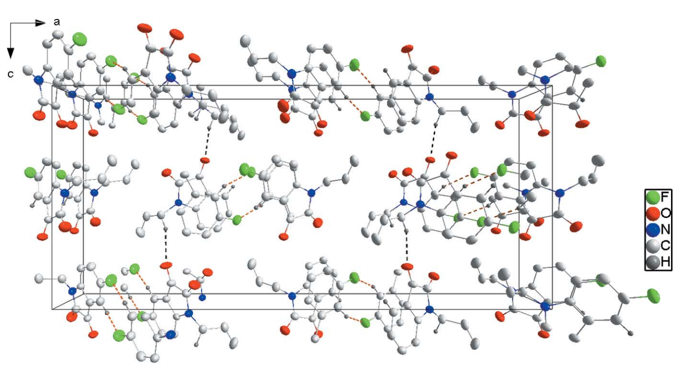


Figure 3
Crystal packing of the title compound viewed along the *b* axis. The C—H⋯F and C—H⋯O hydrogen bonds are shown, respectively, by orange and black dotted lines.

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

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C5—H5⋯F2	0.95	2.64	3.477 (6)	148
C9—H9*B*⋯O1[i]	0.99	2.45	3.408 (7)	163
C16—H16⋯F1	0.95	2.50	3.353 (5)	150

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{11}H_8FNO_2$
M_r	205.18
Crystal system, space group	Orthorhombic, $Pna2_1$
Temperature (K)	150
a, b, c (Å)	31.531 (3), 4.2752 (4), 14.1080 (13)
V (Å^3)	1901.8 (3)
Z	8
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.96
Crystal size (mm)	0.27 × 0.07 × 0.06
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.76, 0.94
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13399, 3201, 2813
R_{int}	0.047
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.619
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.073, 0.189, 1.10
No. of reflections	3201
No. of parameters	272
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.86, −0.32
Absolute structure	Refined as an inversion twin
Absolute structure parameter	0.5 (4)

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*) and *DIAMOND* (Brandenburg & Putz, 2012).

Synthesis and crystallization

To a solution of 5-fluoro-2,3-indoledione (0.5 g, 3.5 mmol) dissolved in DMF (20 ml) was added potassium carbonate (0.61 g, 4.4 mmol), a catalytic quantity of tetra-*n*-butylammonium (0.1 g, 0.4 mmol) and 3-bromo-1-propene (0.2 ml, 3.6 mmol). The mixture was stirred for 48 h; the reaction was monitored by thin layer chromatography. The mixture was filtered and the solvent removed under vacuum. The solid obtained was recrystallized from ethanol solution to afford the title compound as red crystals in 86% yield (m.p.: 450 K).

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x170028 [https://doi.org/10.1107/S2414314617000281]

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Crystal data

$C_{11}H_8FNO_2$
M_r = 205.18
Orthorhombic, $Pna2_1$
a = 31.531 (3) Å
b = 4.2752 (4) Å
c = 14.1080 (13) Å
V = 1901.8 (3) Å^3
Z = 8
F(000) = 848
D_x = 1.433 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54178 Å
Cell parameters from 9630 reflections
θ = 3.4–72.5°
μ = 0.96 mm^{-1}
T = 150 K
Column, orange
0.27 × 0.07 × 0.06 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC I*μ*S micro-focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.76, T_{max} = 0.94
13399 measured reflections
3201 independent reflections
2813 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 72.6°, θ_{min} = 2.8°
h = −35→38
k = −5→5
l = −17→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.073
$wR(F^2)$ = 0.189
S = 1.10
3201 reflections
272 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.1367P)^2 + 0.156P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.86 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Absolute structure: Refined as an inversion twin
Absolute structure parameter: 0.5 (4)

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 $F^2 > 2sigma(F^2)$ 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. The model was refined as a 2-component inversion twin.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
F1	0.36220 (9)	0.5663 (7)	0.6091 (3)	0.0471 (8)
O1	0.28379 (13)	1.1914 (11)	0.3187 (3)	0.0519 (10)
O2	0.21272 (12)	1.5827 (9)	0.3844 (3)	0.0466 (9)
N1	0.23084 (11)	1.3640 (9)	0.5286 (3)	0.0296 (8)
C1	0.26289 (13)	1.1603 (10)	0.5611 (3)	0.0268 (9)
C2	0.27104 (14)	1.0662 (10)	0.6529 (3)	0.0308 (9)
H2	0.2540	1.1363	0.7041	0.037*
C3	0.30516 (14)	0.8649 (10)	0.6680 (3)	0.0344 (10)
H3	0.3119	0.7975	0.7304	0.041*
C4	0.32926 (12)	0.7631 (10)	0.5915 (4)	0.0320 (9)
C5	0.32217 (13)	0.8575 (10)	0.4997 (3)	0.0323 (9)
H5	0.3396	0.7889	0.4489	0.039*
C6	0.28839 (13)	1.0576 (10)	0.4855 (3)	0.0291 (9)
C7	0.27201 (14)	1.2069 (11)	0.4003 (3)	0.0320 (9)
C8	0.23410 (14)	1.4111 (11)	0.4335 (4)	0.0348 (10)
C9	0.19819 (13)	1.5140 (9)	0.5867 (4)	0.0323 (9)
H9A	0.1905	1.7172	0.5578	0.039*
H9B	0.2099	1.5561	0.6505	0.039*
C10	0.15888 (13)	1.3173 (10)	0.5963 (4)	0.0371 (10)
H10	0.1456	1.2464	0.5398	0.044*
C11	0.14177 (16)	1.2374 (14)	0.6771 (5)	0.0514 (14)
H11A	0.1542	1.3042	0.7349	0.062*
H11B	0.1169	1.1123	0.6779	0.062*
F2	0.38964 (10)	0.3522 (8)	0.3790 (3)	0.0540 (9)
O3	0.46219 (11)	−0.2464 (9)	0.6830 (3)	0.0463 (9)
O4	0.53563 (12)	−0.6362 (10)	0.6272 (3)	0.0541 (10)
N2	0.52058 (11)	−0.4257 (8)	0.4808 (3)	0.0313 (8)
C12	0.48881 (13)	−0.2282 (9)	0.4430 (3)	0.0255 (8)
C13	0.48270 (14)	−0.1402 (10)	0.3493 (3)	0.0321 (9)
H13	0.5010	−0.2114	0.3003	0.039*
C14	0.44864 (15)	0.0568 (10)	0.3302 (4)	0.0373 (10)
H14	0.4433	0.1198	0.2667	0.045*
C15	0.42247 (13)	0.1622 (10)	0.4021 (4)	0.0353 (10)
C16	0.42799 (13)	0.0785 (10)	0.4950 (4)	0.0343 (10)

H16	0.4096	0.1516	0.5435	0.041*
C17	0.46198 (13)	−0.1195 (10)	0.5149 (3)	0.0320 (9)
C18	0.47587 (13)	−0.2635 (10)	0.6037 (4)	0.0325 (10)
C19	0.51490 (15)	−0.4685 (11)	0.5751 (3)	0.0361 (10)
C20	0.55462 (13)	−0.5753 (10)	0.4267 (4)	0.0351 (10)
H20A	0.5436	−0.6369	0.3637	0.042*
H20B	0.5636	−0.7680	0.4600	0.042*
C21	0.59237 (14)	−0.3680 (10)	0.4134 (4)	0.0377 (11)
H21	0.6048	−0.2783	0.4683	0.045*
C22	0.60947 (17)	−0.3015 (16)	0.3314 (5)	0.0569 (16)
H22A	0.5979	−0.3870	0.2749	0.068*
H22B	0.6335	−0.1677	0.3283	0.068*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0423 (15)	0.0477 (15)	0.0515 (19)	0.0148 (12)	−0.0090 (14)	0.0057 (13)
O1	0.055 (2)	0.079 (3)	0.022 (2)	0.018 (2)	0.0040 (16)	0.0009 (17)
O2	0.050 (2)	0.056 (2)	0.033 (2)	0.0138 (17)	−0.0089 (17)	0.0035 (16)
N1	0.0287 (16)	0.0353 (18)	0.025 (2)	0.0031 (14)	0.0008 (14)	−0.0018 (14)
C1	0.0263 (19)	0.0320 (19)	0.022 (2)	−0.0063 (15)	−0.0031 (16)	−0.0022 (16)
C2	0.031 (2)	0.0341 (19)	0.027 (2)	−0.0034 (16)	0.0029 (17)	−0.0009 (17)
C3	0.037 (2)	0.036 (2)	0.030 (3)	−0.0063 (17)	−0.0061 (19)	0.0079 (18)
C4	0.0248 (19)	0.038 (2)	0.033 (3)	0.0034 (16)	−0.0020 (18)	0.0000 (18)
C5	0.031 (2)	0.0353 (19)	0.031 (2)	−0.0015 (16)	0.0010 (18)	0.0005 (17)
C6	0.0294 (19)	0.0333 (19)	0.024 (2)	−0.0012 (16)	0.0004 (17)	−0.0032 (16)
C7	0.035 (2)	0.040 (2)	0.021 (2)	0.0041 (17)	−0.0011 (19)	−0.0005 (18)
C8	0.035 (2)	0.042 (2)	0.028 (2)	0.0022 (18)	−0.0030 (18)	0.0015 (18)
C9	0.0276 (19)	0.0323 (19)	0.037 (3)	0.0016 (16)	0.0012 (18)	−0.0080 (18)
C10	0.0266 (19)	0.037 (2)	0.047 (3)	0.0012 (16)	−0.004 (2)	−0.007 (2)
C11	0.035 (3)	0.062 (3)	0.057 (4)	−0.006 (2)	0.015 (3)	0.000 (3)
F2	0.0416 (15)	0.0552 (17)	0.065 (2)	0.0140 (13)	−0.0024 (16)	0.0120 (16)
O3	0.043 (2)	0.071 (2)	0.0246 (19)	−0.0072 (17)	0.0022 (15)	−0.0020 (16)
O4	0.047 (2)	0.065 (2)	0.050 (3)	0.0056 (18)	−0.0079 (18)	0.020 (2)
N2	0.0299 (17)	0.0325 (17)	0.031 (2)	0.0008 (14)	−0.0008 (15)	0.0043 (15)
C12	0.0266 (19)	0.0279 (18)	0.022 (2)	−0.0018 (15)	0.0007 (16)	0.0006 (14)
C13	0.033 (2)	0.0325 (19)	0.031 (2)	−0.0047 (16)	0.0009 (18)	0.0009 (18)
C14	0.038 (2)	0.039 (2)	0.035 (2)	−0.0023 (18)	−0.001 (2)	0.0113 (19)
C15	0.026 (2)	0.038 (2)	0.042 (3)	−0.0021 (16)	−0.0081 (19)	0.005 (2)
C16	0.0306 (19)	0.0346 (19)	0.038 (3)	−0.0020 (17)	0.0015 (19)	−0.0027 (17)
C17	0.031 (2)	0.0333 (19)	0.031 (2)	−0.0041 (16)	0.0012 (18)	−0.0031 (17)
C18	0.029 (2)	0.044 (2)	0.025 (2)	−0.0069 (16)	−0.0004 (19)	0.0019 (18)
C19	0.037 (2)	0.043 (2)	0.029 (2)	−0.0033 (18)	−0.0045 (17)	0.0037 (19)
C20	0.031 (2)	0.0313 (19)	0.043 (3)	0.0017 (16)	0.0002 (19)	−0.0058 (18)
C21	0.027 (2)	0.033 (2)	0.053 (3)	0.0015 (17)	−0.003 (2)	−0.003 (2)
C22	0.039 (3)	0.068 (4)	0.063 (4)	−0.009 (2)	0.009 (3)	−0.005 (3)

Geometric parameters (Å, º)

F1—C4	1.360 (5)	F2—C15	1.355 (5)
O1—C7	1.212 (6)	O3—C18	1.202 (6)
O2—C8	1.213 (6)	O4—C19	1.217 (6)
N1—C8	1.362 (6)	N2—C19	1.356 (6)
N1—C1	1.411 (5)	N2—C12	1.414 (5)
N1—C9	1.463 (5)	N2—C20	1.464 (6)
C1—C2	1.380 (6)	C12—C13	1.388 (7)
C1—C6	1.406 (6)	C12—C17	1.400 (6)
C2—C3	1.394 (6)	C13—C14	1.391 (6)
C2—H2	0.9500	C13—H13	0.9500
C3—C4	1.389 (7)	C14—C15	1.383 (7)
C3—H3	0.9500	C14—H14	0.9500
C4—C5	1.375 (7)	C15—C16	1.370 (7)
C5—C6	1.381 (6)	C16—C17	1.394 (6)
C5—H5	0.9500	C16—H16	0.9500
C6—C7	1.456 (6)	C17—C18	1.463 (7)
C7—C8	1.552 (6)	C18—C19	1.564 (6)
C9—C10	1.504 (6)	C20—C21	1.496 (6)
C9—H9A	0.9900	C20—H20A	0.9900
C9—H9B	0.9900	C20—H20B	0.9900
C10—C11	1.306 (8)	C21—C22	1.307 (8)
C10—H10	0.9500	C21—H21	0.9500
C11—H11A	0.9500	C22—H22A	0.9500
C11—H11B	0.9500	C22—H22B	0.9500
C8—N1—C1	110.9 (4)	C19—N2—C12	110.9 (4)
C8—N1—C9	122.7 (4)	C19—N2—C20	123.4 (4)
C1—N1—C9	126.4 (4)	C12—N2—C20	125.7 (4)
C2—C1—C6	120.9 (4)	C13—C12—C17	121.1 (4)
C2—C1—N1	128.2 (4)	C13—C12—N2	128.2 (4)
C6—C1—N1	110.9 (4)	C17—C12—N2	110.7 (4)
C1—C2—C3	117.9 (4)	C12—C13—C14	117.1 (4)
C1—C2—H2	121.1	C12—C13—H13	121.4
C3—C2—H2	121.1	C14—C13—H13	121.4
C4—C3—C2	119.8 (4)	C15—C14—C13	121.0 (5)
C4—C3—H3	120.1	C15—C14—H14	119.5
C2—C3—H3	120.1	C13—C14—H14	119.5
F1—C4—C5	118.5 (4)	F2—C15—C16	118.9 (4)
F1—C4—C3	118.0 (4)	F2—C15—C14	118.3 (5)
C5—C4—C3	123.4 (4)	C16—C15—C14	122.7 (4)
C4—C5—C6	116.4 (4)	C15—C16—C17	116.7 (4)
C4—C5—H5	121.8	C15—C16—H16	121.7
C6—C5—H5	121.8	C17—C16—H16	121.7
C5—C6—C1	121.6 (4)	C16—C17—C12	121.4 (4)
C5—C6—C7	131.7 (4)	C16—C17—C18	131.1 (4)
C1—C6—C7	106.7 (4)	C12—C17—C18	107.4 (4)

O1—C7—C6	130.7 (4)	O3—C18—C17	131.6 (4)
O1—C7—C8	123.6 (4)	O3—C18—C19	123.8 (4)
C6—C7—C8	105.7 (4)	C17—C18—C19	104.5 (4)
O2—C8—N1	127.6 (5)	O4—C19—N2	126.9 (5)
O2—C8—C7	126.6 (5)	O4—C19—C18	126.7 (5)
N1—C8—C7	105.8 (4)	N2—C19—C18	106.3 (4)
N1—C9—C10	112.7 (3)	N2—C20—C21	113.0 (3)
N1—C9—H9A	109.1	N2—C20—H20A	109.0
C10—C9—H9A	109.1	C21—C20—H20A	109.0
N1—C9—H9B	109.1	N2—C20—H20B	109.0
C10—C9—H9B	109.1	C21—C20—H20B	109.0
H9A—C9—H9B	107.8	H20A—C20—H20B	107.8
C11—C10—C9	124.5 (5)	C22—C21—C20	124.6 (5)
C11—C10—H10	117.8	C22—C21—H21	117.7
C9—C10—H10	117.8	C20—C21—H21	117.7
C10—C11—H11A	120.0	C21—C22—H22A	120.0
C10—C11—H11B	120.0	C21—C22—H22B	120.0
H11A—C11—H11B	120.0	H22A—C22—H22B	120.0

C8—N1—C1—C2	177.3 (4)	C19—N2—C12—C13	−177.0 (4)
C9—N1—C1—C2	−1.9 (7)	C20—N2—C12—C13	1.2 (7)
C8—N1—C1—C6	−1.5 (5)	C19—N2—C12—C17	3.3 (5)
C9—N1—C1—C6	179.3 (4)	C20—N2—C12—C17	−178.5 (4)
C6—C1—C2—C3	−0.4 (6)	C17—C12—C13—C14	−0.7 (6)
N1—C1—C2—C3	−179.1 (4)	N2—C12—C13—C14	179.6 (4)
C1—C2—C3—C4	−0.8 (6)	C12—C13—C14—C15	0.8 (6)
C2—C3—C4—F1	−179.8 (4)	C13—C14—C15—F2	−179.6 (4)
C2—C3—C4—C5	1.9 (7)	C13—C14—C15—C16	−0.7 (7)
F1—C4—C5—C6	−179.9 (4)	F2—C15—C16—C17	179.4 (4)
C3—C4—C5—C6	−1.7 (6)	C14—C15—C16—C17	0.5 (6)
C4—C5—C6—C1	0.4 (6)	C15—C16—C17—C12	−0.5 (6)
C4—C5—C6—C7	178.9 (4)	C15—C16—C17—C18	−177.0 (4)
C2—C1—C6—C5	0.6 (6)	C13—C12—C17—C16	0.6 (6)
N1—C1—C6—C5	179.5 (4)	N2—C12—C17—C16	−179.7 (4)
C2—C1—C6—C7	−178.2 (4)	C13—C12—C17—C18	177.9 (4)
N1—C1—C6—C7	0.7 (5)	N2—C12—C17—C18	−2.4 (5)
C5—C6—C7—O1	0.8 (9)	C16—C17—C18—O3	−1.3 (8)
C1—C6—C7—O1	179.4 (5)	C12—C17—C18—O3	−178.2 (5)
C5—C6—C7—C8	−178.4 (4)	C16—C17—C18—C19	177.7 (4)
C1—C6—C7—C8	0.3 (5)	C12—C17—C18—C19	0.8 (4)
C1—N1—C8—O2	−176.7 (5)	C12—N2—C19—O4	176.5 (5)
C9—N1—C8—O2	2.5 (8)	C20—N2—C19—O4	−1.8 (7)
C1—N1—C8—C7	1.6 (5)	C12—N2—C19—C18	−2.6 (5)
C9—N1—C8—C7	−179.2 (4)	C20—N2—C19—C18	179.1 (4)
O1—C7—C8—O2	−2.1 (8)	O3—C18—C19—O4	1.1 (8)
C6—C7—C8—O2	177.1 (5)	C17—C18—C19—O4	−178.0 (5)
O1—C7—C8—N1	179.6 (5)	O3—C18—C19—N2	−179.8 (4)
C6—C7—C8—N1	−1.1 (5)	C17—C18—C19—N2	1.1 (5)

C8—N1—C9—C10	91.9 (5)	C19—N2—C20—C21	−97.0 (5)
C1—N1—C9—C10	−89.0 (5)	C12—N2—C20—C21	85.0 (5)
N1—C9—C10—C11	125.9 (5)	N2—C20—C21—C22	−126.1 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···F2	0.95	2.64	3.477 (6)	148
C9—H9*B*···O1[i]	0.99	2.45	3.408 (7)	163
C16—H16···F1	0.95	2.50	3.353 (5)	150

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