Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Ethyl 2-amino-4,6-bis(4-fluorophenyl)-cyclohexa-1,3-diene-1-carboxylate

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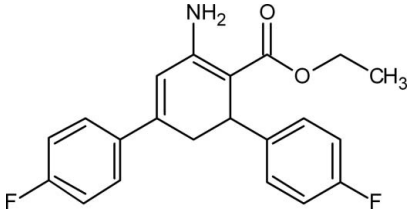
Received 30 December 2011; accepted 27 January 2012

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.055; wR factor = 0.180; data-to-parameter ratio = 14.1.

In the title compound, $C_{21}H_{19}F_2NO_2$, the cyclohexa-1,3-diene ring is in a distorted envelope conformation. The dihedral angles between the mean planes of the diene moiety and the two fluorophenyl rings are 42.8 (2) and 75.0 (5)°. The two fluorophenyl rings are inclined to one another by 87.0 (3)°. In the crystal, intramolecular N—H···O hydrogen bonds and weak N—H···O and N—H···F intermolecular interactions are observed forming an infinite two-dimensional network along [011].

Related literature

For background to the applications of cyclohexenones, see: Padmavathi *et al.* (1999, 2000); Padmavathi, Sharmila, Balaiah *et al.* (2001); Padmavathi, Sharmila, Somashekara Reddy & Bhaskar Reddy (2001). For the structure of the precursor of the title compound, see: Dutkiewicz *et al.* (2011). For various derivatives of 4,4-difluorochalcone, see: Fun *et al.* (2010*a*,*b*); Jasinski *et al.* (2010*a*,*b*). For puckering parameters, see: Cremer & Pople (1975).



Experimental

Crystal data

$C_{21}H_{19}F_2NO_2$
M_r = 355.37
Orthorhombic, *Pbcn*
a = 18.0199 (5) Å
b = 9.6391 (2) Å
c = 21.0754 (7) Å
V = 3660.70 (18) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 0.80 mm^{-1}
T = 173 K
0.20 × 0.14 × 0.12 mm

Data collection

Oxford Xcalibur Eos Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2010)
T_{min} = 0.856, T_{max} = 0.910
10556 measured reflections
3461 independent reflections
2612 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.180
S = 1.04
3461 reflections
245 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1B···O2^{i}	0.86 (3)	2.23 (3)	3.066 (2)	165 (2)
N1—H1A···O2	0.88 (2)	2.06 (2)	2.708 (2)	130.3 (19)
N1—H1A···F1^{ii}	0.88 (2)	2.37 (2)	3.104 (2)	141.9 (19)

Symmetry codes: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, z$; (ii) $x+\frac{1}{2}, -y+\frac{1}{2}, -z+1$.

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

HSY thanks the University of Mysore for research facilities. JPJ acknowledges the NSF–MRI program (grant No. CHE1039027) for funds to purchase the X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: MW2046).

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supplementary materials

Acta Cryst. (2012). E**68**, o585 [doi:10.1107/S160053681200373X]

Ethyl 2-amino-4,6-bis(4-fluorophenyl)cyclohexa-1,3-diene-1-carboxylate

Jerry P. Jasinski, James A. Golen, S. Samshuddin, B. Narayana and H. S. Yathirajan

Comment

Cyclohexenones are efficient synthons in building spiro compounds (Padmavathi, Sharmila, Somashekara Reddy & Bhaskar Reddy, 2001) or intermediates in the synthesis of benzisoxazoles or carbazole derivatives (Padmavathi *et al.*, 1999, 2000; Padmavathi, Sharmila, Balaiah *et al.*, 2001). The cyclohexenone derivative of 4,4-difluorochalcone reacts with ammonium acetate to yield the title compound (I). The crystal structure of (1RS,6SR)-ethyl 4,6-bis(4-fluorophenyl)-2-oxocyclohex-3-ene-1-carboxylate, which is the precursor of the title compound (I), has been reported (Dutkiewicz *et al.*, 2011). In continuation of our work on the synthesis of various derivatives of 4,4-difluorochalcone (Fun *et al.*, 2010*a*,*b*; Jasinski *et al.*, 2010*a*,*b*), the title compound, (I), was synthesized and its crystal structure is reported here.

In the title compound, $C_{21}H_{19}F_2NO_2$, the 1,3-cyclohexadiene ring is in a distorted envelope conformation with Cremer & Pople puckering parameters Q, θ and φ of 0.389 (2) Å, 115.8 (3)° and 90.9 (4)° (Cremer & Pople, 1975). For an ideal envelope conformation θ and φ are 54.7° and 120°. The dihedral angles between the mean planes of the diene moiety (C4/C3/O2/O1) and the two fluorophenyl rings are 42.8 (2)° and 75.0 (5)°, respectively (Fig. 1). The two fluorophenyl rings are inclined to one another by 87.0 (3)°. Intramolecular N—H···O hydrogen bonds and weak N—H···O, N—H···F intermolecular interactions (Table 1) are observed forming an infinite 2-D network along [011] (Fig. 2).

Experimental

A mixture of ethyl 4,6-bis(4-fluorophenyl)-2-oxocyclohex-3-ene-1-carboxylate (3.55 g, 0.01 mol) and ammonim acetate (0.77g, 0.01 mol) in 20 ml of ethanol was refluxed for 10 h. The reaction mixture was cooled and poured into 50 ml of ice-cold water. The precipitate was collected by filtration and purified by recrystallization from ethanol. Single crystals were grown from DMF by the slow evaporation method and the yield of the compound was 70%. (m.p. 428 K).

Refinement

H1A and H1B were located by a difference map and refined isotropically. All of the remaining H atoms were placed in their calculated positions and then refined using the riding model with atom—H lengths of 0.95 Å (CH), 0.99 Å (CH_2) or 0.98 Å (CH_3). Isotropic displacement parameters for these atoms were set to 1.2 (CH, CH_2) or 1.5 (CH_3) times U_{eq} of the parent atom.

Computing details

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO* (Oxford Diffraction, 2010); data reduction: *CrysAlis RED* (Oxford Diffraction, 2010); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

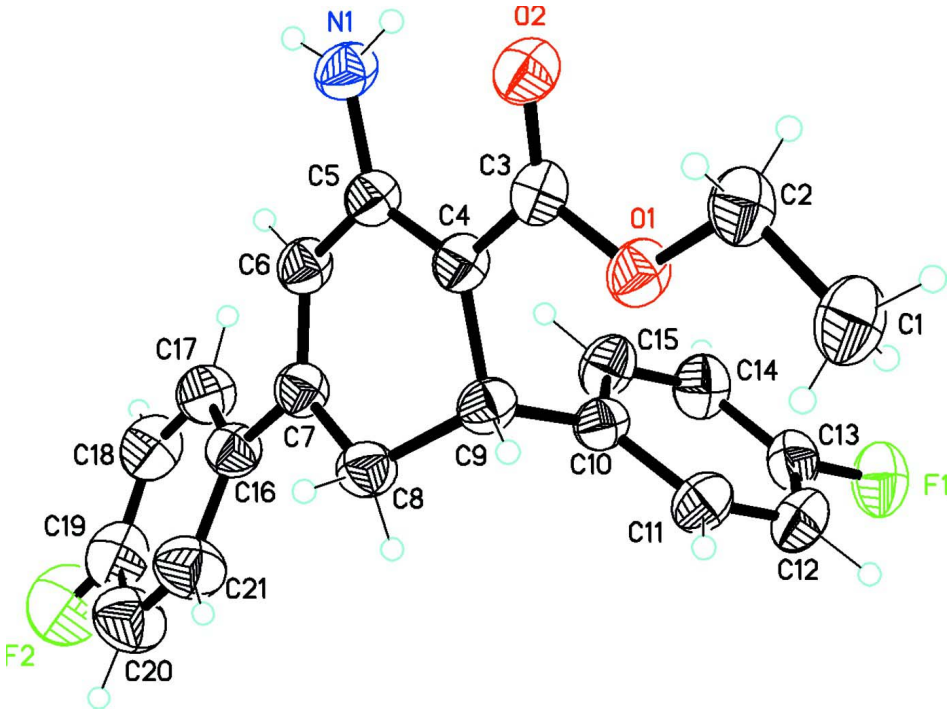

Figure 1

Molecular structure of the title compound showing the atom labeling scheme and 50% probability displacement ellipsoids.

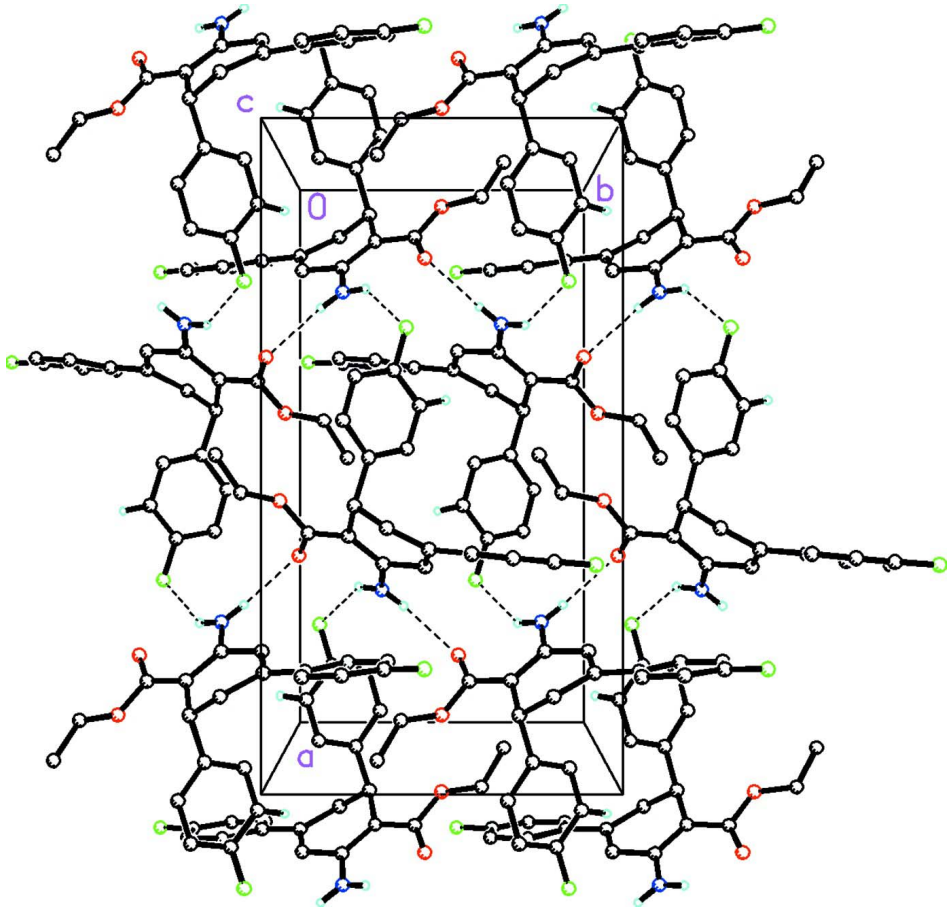

Figure 2

Packing diagram of the title compound viewed along the *c* axis. Dashed lines indicate N—H···O intramolecular hydrogen bonds and weak N—H···O, N—H···F intermolecular interactions forming an infinite 2-D network along [011]. Remaining H atoms have been removed for clarity.

Ethyl 2-amino-4,6-bis(4-fluorophenyl)cyclohexa-1,3-diene-1-carboxylate

Crystal data

$C_{21}H_{19}F_2NO_2$
$M_r = 355.37$
Orthorhombic, *Pbcn*
Hall symbol: -P 2n 2ab
$a = 18.0199\ (5)$ Å
$b = 9.6391\ (2)$ Å
$c = 21.0754\ (7)$ Å
$V = 3660.70\ (18)$ Å^3
$Z = 8$
$F(000) = 1488$
$D_x = 1.290$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 4418 reflections
$\theta = 3.2–71.3°$
$\mu = 0.80$ mm^{-1}
$T = 173$ K
Block, yellow
0.20 × 0.14 × 0.12 mm

Data collection

Oxford Xcalibur Eos Gemini diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 16.1500 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2010)
$T_{min} = 0.856$, $T_{max} = 0.910$
10556 measured reflections

3461 independent reflections
2612 reflections with $I > 2\sigma(I)$
$R_{int} = 0.017$
$\theta_{max} = 71.4°$, $\theta_{min} = 4.2°$
$h = -21 \rightarrow 16$
$k = -11 \rightarrow 11$
$l = -22 \rightarrow 25$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.180$
$S = 1.04$
3461 reflections
245 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
$w = 1/[\sigma^2(F_o^2) + (0.1072P)^2 + 0.4506P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0010 (2)

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}
F1	0.28820 (7)	0.39132 (16)	0.58085 (8)	0.0963 (5)
F2	0.66890 (12)	0.94956 (19)	0.80642 (12)	0.1445 (8)
O1	0.57361 (8)	0.00028 (13)	0.57519 (7)	0.0679 (4)
O2	0.66652 (8)	0.05261 (14)	0.50837 (8)	0.0695 (4)
N1	0.72288 (11)	0.3120 (2)	0.51875 (9)	0.0692 (5)
H1B	0.7509 (15)	0.380 (3)	0.5083 (10)	0.076 (7)*
H1A	0.7197 (12)	0.239 (2)	0.4942 (11)	0.066 (6)*
C1	0.49783 (15)	−0.1988 (2)	0.57203 (16)	0.0931 (8)
H1C	0.4854	−0.2832	0.5484	0.140*
H1D	0.4545	−0.1375	0.5734	0.140*
H1E	0.5124	−0.2235	0.6154	0.140*
C2	0.56045 (13)	−0.12602 (19)	0.53997 (12)	0.0746 (6)
H2A	0.6054	−0.1850	0.5401	0.089*
H2B	0.5473	−0.1043	0.4954	0.089*
C3	0.62737 (10)	0.08577 (18)	0.55369 (10)	0.0578 (5)
C4	0.63143 (11)	0.21328 (19)	0.58891 (10)	0.0572 (5)
C5	0.67799 (11)	0.31852 (19)	0.56986 (10)	0.0572 (5)
C6	0.68054 (11)	0.44920 (19)	0.60540 (10)	0.0609 (5)
H6A	0.7040	0.5274	0.5867	0.073*
C7	0.65069 (11)	0.4618 (2)	0.66361 (10)	0.0600 (5)

C8	0.61518 (13)	0.3357 (2)	0.69326 (10)	0.0667 (5)
H8A	0.5763	0.3668	0.7232	0.080*
H8B	0.6532	0.2852	0.7181	0.080*
C9	0.58026 (11)	0.23520 (19)	0.64523 (10)	0.0592 (5)
H9A	0.5759	0.1435	0.6671	0.071*
C10	0.50212 (11)	0.27746 (17)	0.62632 (9)	0.0559 (5)
C11	0.44170 (12)	0.2002 (2)	0.64594 (11)	0.0684 (6)
H11A	0.4499	0.1195	0.6709	0.082*
C12	0.37006 (13)	0.2363 (2)	0.63060 (12)	0.0770 (6)
H12A	0.3293	0.1813	0.6443	0.092*
C13	0.35890 (12)	0.3530 (2)	0.59515 (11)	0.0690 (6)
C14	0.41611 (13)	0.4322 (2)	0.57387 (12)	0.0748 (6)
H14A	0.4070	0.5126	0.5490	0.090*
C15	0.48779 (12)	0.3937 (2)	0.58902 (11)	0.0715 (6)
H15A	0.5281	0.4476	0.5737	0.086*
C16	0.65610 (11)	0.5913 (2)	0.70079 (11)	0.0648 (5)
C17	0.66870 (14)	0.7180 (2)	0.67350 (13)	0.0781 (6)
H17A	0.6753	0.7226	0.6288	0.094*
C18	0.67220 (15)	0.8387 (3)	0.70790 (17)	0.0898 (8)
H18A	0.6790	0.9256	0.6874	0.108*
C19	0.66577 (16)	0.8309 (3)	0.77206 (18)	0.0979 (9)
C20	0.6589 (2)	0.7078 (3)	0.80307 (16)	0.1065 (10)
H20A	0.6580	0.7039	0.8481	0.128*
C21	0.65327 (18)	0.5888 (3)	0.76701 (13)	0.0934 (8)
H21A	0.6473	0.5023	0.7879	0.112*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0684 (8)	0.0980 (10)	0.1224 (13)	0.0017 (7)	−0.0188 (8)	−0.0061 (8)
F2	0.1599 (17)	0.0981 (12)	0.175 (2)	−0.0024 (11)	0.0216 (15)	−0.0716 (13)
O1	0.0700 (8)	0.0498 (7)	0.0838 (10)	−0.0096 (6)	0.0083 (7)	−0.0045 (6)
O2	0.0641 (8)	0.0553 (7)	0.0891 (11)	0.0019 (6)	0.0118 (8)	−0.0099 (7)
N1	0.0711 (11)	0.0588 (10)	0.0776 (13)	−0.0125 (8)	0.0186 (10)	−0.0101 (9)
C1	0.0954 (18)	0.0609 (12)	0.123 (2)	−0.0220 (12)	0.0001 (16)	0.0023 (13)
C2	0.0793 (14)	0.0475 (10)	0.0970 (17)	−0.0052 (9)	−0.0028 (12)	−0.0052 (10)
C3	0.0523 (9)	0.0474 (9)	0.0737 (13)	0.0016 (7)	−0.0012 (10)	0.0031 (8)
C4	0.0568 (10)	0.0500 (9)	0.0646 (12)	−0.0010 (8)	0.0013 (9)	0.0002 (8)
C5	0.0565 (10)	0.0524 (9)	0.0627 (12)	−0.0008 (8)	0.0039 (9)	−0.0009 (8)
C6	0.0622 (11)	0.0510 (9)	0.0696 (13)	−0.0085 (8)	0.0040 (10)	−0.0006 (8)
C7	0.0620 (11)	0.0568 (10)	0.0613 (12)	−0.0023 (8)	−0.0005 (9)	−0.0001 (8)
C8	0.0737 (13)	0.0658 (11)	0.0607 (12)	−0.0078 (9)	0.0050 (10)	0.0020 (9)
C9	0.0644 (11)	0.0490 (9)	0.0642 (12)	−0.0044 (8)	0.0068 (9)	0.0062 (8)
C10	0.0627 (11)	0.0452 (8)	0.0598 (11)	−0.0051 (8)	0.0086 (9)	−0.0033 (7)
C11	0.0690 (12)	0.0577 (11)	0.0784 (14)	−0.0072 (9)	0.0090 (11)	0.0090 (9)
C12	0.0653 (12)	0.0725 (13)	0.0932 (17)	−0.0160 (10)	0.0096 (12)	0.0049 (12)
C13	0.0622 (12)	0.0663 (12)	0.0786 (14)	0.0002 (9)	−0.0066 (11)	−0.0128 (10)
C14	0.0780 (14)	0.0578 (11)	0.0886 (16)	−0.0029 (10)	−0.0080 (12)	0.0086 (10)
C15	0.0680 (13)	0.0568 (11)	0.0897 (16)	−0.0090 (9)	0.0015 (11)	0.0141 (10)
C16	0.0651 (11)	0.0623 (11)	0.0671 (13)	0.0023 (9)	0.0036 (10)	−0.0047 (9)

C17	0.0852 (15)	0.0661 (13)	0.0831 (16)	−0.0069 (10)	0.0037 (12)	−0.0076 (11)
C18	0.0873 (17)	0.0642 (13)	0.118 (2)	−0.0003 (11)	0.0098 (16)	−0.0136 (14)
C19	0.0881 (18)	0.0780 (16)	0.128 (3)	0.0035 (13)	0.0108 (16)	−0.0422 (16)
C20	0.129 (3)	0.098 (2)	0.092 (2)	0.0000 (17)	0.0041 (18)	−0.0281 (16)
C21	0.119 (2)	0.0792 (15)	0.0816 (18)	−0.0014 (14)	0.0062 (15)	−0.0085 (13)

Geometric parameters (Å, º)

F1—C13	1.360 (2)	C8—H8B	0.9900
F2—C19	1.355 (3)	C9—C10	1.519 (3)
O1—C3	1.350 (2)	C9—H9A	1.0000
O1—C2	1.445 (2)	C10—C11	1.382 (3)
O2—C3	1.230 (2)	C10—C15	1.393 (3)
N1—C5	1.348 (3)	C11—C12	1.375 (3)
N1—H1B	0.86 (3)	C11—H11A	0.9500
N1—H1A	0.88 (2)	C12—C13	1.366 (3)
C1—C2	1.491 (3)	C12—H12A	0.9500
C1—H1C	0.9800	C13—C14	1.359 (3)
C1—H1D	0.9800	C14—C15	1.381 (3)
C1—H1E	0.9800	C14—H14A	0.9500
C2—H2A	0.9900	C15—H15A	0.9500
C2—H2B	0.9900	C16—C17	1.369 (3)
C3—C4	1.438 (3)	C16—C21	1.397 (4)
C4—C5	1.376 (3)	C17—C18	1.372 (3)
C4—C9	1.518 (3)	C17—H17A	0.9500
C5—C6	1.466 (3)	C18—C19	1.359 (5)
C6—C7	1.345 (3)	C18—H18A	0.9500
C6—H6A	0.9500	C19—C20	1.360 (4)
C7—C16	1.478 (3)	C20—C21	1.379 (4)
C7—C8	1.508 (3)	C20—H20A	0.9500
C8—C9	1.536 (3)	C21—H21A	0.9500
C8—H8A	0.9900		
C3—O1—C2	117.35 (16)	C4—C9—H9A	106.6
C5—N1—H1B	121.5 (15)	C10—C9—H9A	106.6
C5—N1—H1A	118.0 (15)	C8—C9—H9A	106.6
H1B—N1—H1A	120 (2)	C11—C10—C15	117.13 (19)
C2—C1—H1C	109.5	C11—C10—C9	120.48 (17)
C2—C1—H1D	109.5	C15—C10—C9	122.39 (17)
H1C—C1—H1D	109.5	C12—C11—C10	122.20 (19)
C2—C1—H1E	109.5	C12—C11—H11A	118.9
H1C—C1—H1E	109.5	C10—C11—H11A	118.9
H1D—C1—H1E	109.5	C13—C12—C11	118.4 (2)
O1—C2—C1	106.7 (2)	C13—C12—H12A	120.8
O1—C2—H2A	110.4	C11—C12—H12A	120.8
C1—C2—H2A	110.4	C14—C13—F1	119.0 (2)
O1—C2—H2B	110.4	C14—C13—C12	122.1 (2)
C1—C2—H2B	110.4	F1—C13—C12	118.9 (2)
H2A—C2—H2B	108.6	C13—C14—C15	118.8 (2)
O2—C3—O1	120.91 (17)	C13—C14—H14A	120.6

O2—C3—C4	126.45 (17)	C15—C14—H14A	120.6
O1—C3—C4	112.64 (17)	C14—C15—C10	121.3 (2)
C5—C4—C3	120.69 (18)	C14—C15—H15A	119.3
C5—C4—C9	119.73 (17)	C10—C15—H15A	119.3
C3—C4—C9	119.46 (16)	C17—C16—C21	116.2 (2)
N1—C5—C4	124.37 (18)	C17—C16—C7	122.8 (2)
N1—C5—C6	115.42 (17)	C21—C16—C7	120.8 (2)
C4—C5—C6	120.21 (18)	C16—C17—C18	122.8 (3)
C7—C6—C5	122.06 (17)	C16—C17—H17A	118.6
C7—C6—H6A	119.0	C18—C17—H17A	118.6
C5—C6—H6A	119.0	C19—C18—C17	118.3 (3)
C6—C7—C16	122.23 (18)	C19—C18—H18A	120.8
C6—C7—C8	118.36 (18)	C17—C18—H18A	120.8
C16—C7—C8	119.27 (18)	F2—C19—C18	118.8 (3)
C7—C8—C9	114.13 (17)	F2—C19—C20	118.9 (3)
C7—C8—H8A	108.7	C18—C19—C20	122.3 (2)
C9—C8—H8A	108.7	C19—C20—C21	117.9 (3)
C7—C8—H8B	108.7	C19—C20—H20A	121.1
C9—C8—H8B	108.7	C21—C20—H20A	121.1
H8A—C8—H8B	107.6	C20—C21—C16	122.2 (3)
C4—C9—C10	113.29 (17)	C20—C21—H21A	118.9
C4—C9—C8	110.75 (16)	C16—C21—H21A	118.9
C10—C9—C8	112.54 (17)		

C3—O1—C2—C1	−178.43 (19)	C8—C9—C10—C15	70.1 (2)
C2—O1—C3—O2	−4.5 (3)	C15—C10—C11—C12	−1.0 (3)
C2—O1—C3—C4	175.00 (17)	C9—C10—C11—C12	179.0 (2)
O2—C3—C4—C5	5.9 (3)	C10—C11—C12—C13	−0.5 (4)
O1—C3—C4—C5	−173.59 (18)	C11—C12—C13—C14	1.2 (4)
O2—C3—C4—C9	−177.93 (19)	C11—C12—C13—F1	−178.6 (2)
O1—C3—C4—C9	2.6 (3)	F1—C13—C14—C15	179.4 (2)
C3—C4—C5—N1	−0.6 (3)	C12—C13—C14—C15	−0.5 (4)
C9—C4—C5—N1	−176.69 (19)	C13—C14—C15—C10	−1.1 (4)
C3—C4—C5—C6	178.74 (18)	C11—C10—C15—C14	1.8 (3)
C9—C4—C5—C6	2.6 (3)	C9—C10—C15—C14	−178.2 (2)
N1—C5—C6—C7	−166.7 (2)	C6—C7—C16—C17	22.1 (3)
C4—C5—C6—C7	14.0 (3)	C8—C7—C16—C17	−162.2 (2)
C5—C6—C7—C16	177.17 (19)	C6—C7—C16—C21	−153.7 (2)
C5—C6—C7—C8	1.4 (3)	C8—C7—C16—C21	22.1 (3)
C6—C7—C8—C9	−31.0 (3)	C21—C16—C17—C18	−5.4 (4)
C16—C7—C8—C9	153.08 (18)	C7—C16—C17—C18	178.6 (2)
C5—C4—C9—C10	96.8 (2)	C16—C17—C18—C19	2.7 (4)
C3—C4—C9—C10	−79.4 (2)	C17—C18—C19—F2	−179.8 (2)
C5—C4—C9—C8	−30.7 (3)	C17—C18—C19—C20	2.6 (5)
C3—C4—C9—C8	153.10 (17)	F2—C19—C20—C21	177.8 (3)
C7—C8—C9—C4	43.9 (2)	C18—C19—C20—C21	−4.5 (5)
C7—C8—C9—C10	−84.0 (2)	C19—C20—C21—C16	1.5 (5)
C4—C9—C10—C11	123.5 (2)	C17—C16—C21—C20	3.3 (4)
C8—C9—C10—C11	−109.9 (2)	C7—C16—C21—C20	179.4 (3)

C4—C9—C10—C15	−56.5 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*B*···O2^{i}	0.86 (3)	2.23 (3)	3.066 (2)	165 (2)
N1—H1*A*···O2	0.88 (2)	2.06 (2)	2.708 (2)	130.3 (19)
N1—H1*A*···F1^{ii}	0.88 (2)	2.37 (2)	3.104 (2)	141.9 (19)

Symmetry codes: (i) −*x*+3/2, *y*+1/2, *z*; (ii) *x*+1/2, −*y*+1/2, −*z*+1.