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4-(4-Fluorophenyl)-2-oxo-1,2,5,6-tetrahydrobenzo[*h*]quinoline-3-carbonitrile

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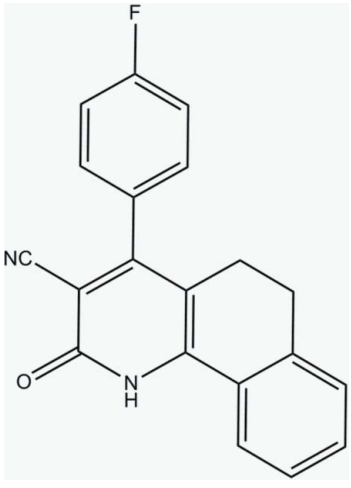
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.048; wR factor = 0.144; data-to-parameter ratio = 11.1.

In the molecule of the title compound, $C_{20}H_{13}FN_2O$, the fluorophenyl ring is oriented at a dihedral angle of 72.76 (3)° with respect to the fused benzene ring. In the crystal structure, intermolecular N—H···O, C—H···O and C—H···F interactions link the molecules into chains. π–π contacts between the quinoline and benzene rings [centroid–centroid distance = 3.918 (3) Å] may further stabilize the structure. A weak C—H···π interaction is also present. The O atom and two of the CH_2 groups of the quinoline ring system are disordered over two positions. The O atom was refined with occupancies of 0.489 (17) and 0.511 (17), while C and H atoms were refined with occupancies of 0.435 (13) and 0.565 (13).

Related literature

For general background to substituted six-membered lactams, see: Daly (1998); Plunkett (1994); Robertson *et al.* (1986). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{20}H_{13}FN_2O$
M_r = 316.32
Triclinic, $P\overline{1}$
a = 8.116 (10) Å
b = 9.278 (12) Å
c = 11.263 (14) Å
α = 98.674 (19)°
β = 105.095 (17)°
γ = 104.846 (18)°
V = 769.7 (16) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 K
0.48 × 0.35 × 0.33 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.956, T_{max} = 0.970
3950 measured reflections
2656 independent reflections
1399 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.144
S = 1.00
2656 reflections
240 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.86	2.08	2.883 (3)	155
C7—H7···O1^{i}	0.93	2.35	3.223 (3)	157
C12—H12*B*···O1^{ii}	0.97	2.21	2.863 (3)	124
C13—H13*B*···F1^{iii}	0.97	2.42	3.270 (3)	147
C15—H15···*Cg*3^{iv}	0.93	2.90	3.671 (3)	141

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2684).

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4-(4-Fluorophenyl)-2-oxo-1,2,5,6-tetrahydrobenzo[*h*]quinoline-3-carbonitrile

Jinpeng Zhang, Jie Ding, Shu Yan, Liangce Rong and Lichun Xu

S1. Comment

Substituted six-membered lactams have attracted the attention of synthetic organic chemists for many years because these structural features are found in a wide variety of naturally occurring alkaloids (Daly, 1998; Plunkett, 1994). Since compounds with these scaffolds have been shown to exhibit significant pharmacological properties, medicinal chemists often incorporate these motifs in the design of novel biologically active molecules. For example, compounds Arnrinone 1 and Milrinone 2 are the cardiotonic drugs (Robertson *et al.*, 1986) and that have been found to display effective activities on therapy of miocardial infarction. Development of a general and efficient synthetic strategy to synthesize those compounds is still desired. We report herein the crystal structure of the title compound.

In the molecule of the title compound (Fig. 1), the bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. Rings A (N1/C1-C5), C (C6-C11) and D (C14-C19) are, of course, planar and they are oriented at dihedral angles of A/C = 3.57 (3), A/D = 76.11 (3) and C/D = 72.76 (3) °. Ring B (C4-C6/C11-C13) is not planar, and adopts twisted conformation.

In the crystal structure, intermolecular N-H···O, C-H···O and C-H···F interactions (Table 1) link the molecules into chains (Fig. 2), in which they may be effective in the stabilization of the structure. The $\pi\cdots\pi$ contact between the quinoline and the benzene rings, Cg1—Cg3^{i} [symmetry code: (i) 1 - x, -y, 1 - z, where Cg1 and Cg3 are centroids of the rings A (N1/C1-C5) and C (C6-C11), respectively] may further stabilize the structure, with centroid-centroid distance of 3.918 (3) Å. There also exists a weak C-H···π interaction (Table 1).

S2. Experimental

The title compound was prepared by the reaction of 3,4-dihydronaphthalen-1(2H) -one (2 mmol), aromatic aldehydes (2 mmol), malononitrile (3 mmol) and NaOH (2 mmol) under solvent-free conditions using heating method.

S3. Refinement

The O1, C12, C13, H12A, H12B, H13A and H13B atoms were disordered. During the refinement process, the disordered C and H atoms were refined with occupancies of 0.435 (13) and 0.565 (13), while O atom was refined with occupancies of 0.489 (17) and 0.511 (17). H atoms were positioned geometrically with N-H = 0.86 Å (for NH) and C-H = 0.93 and 0.97 Å, for aromatic and methylene H atoms, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C,N).

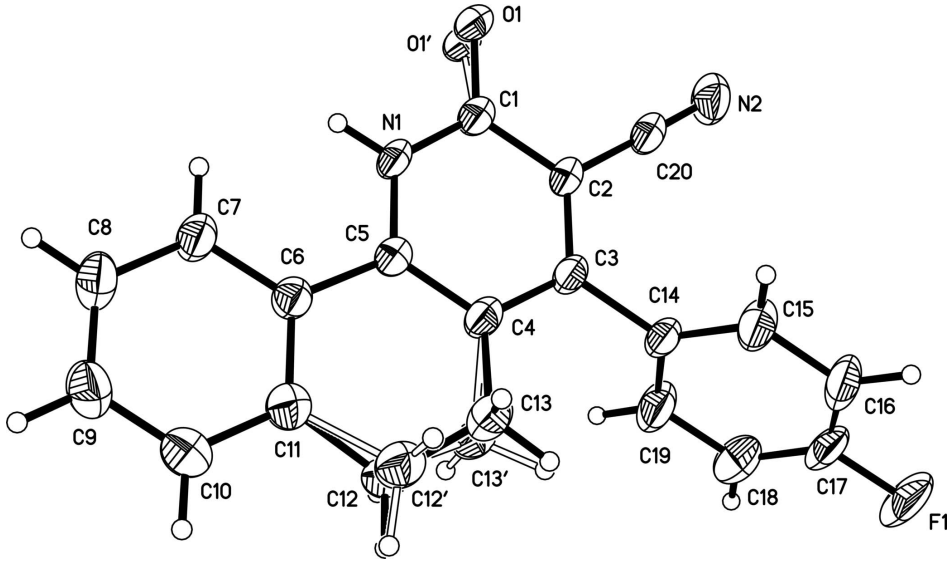

Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

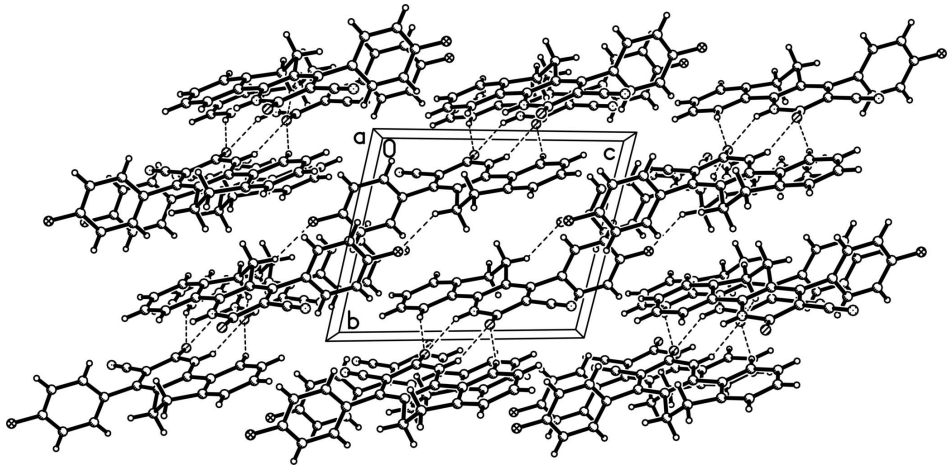

Figure 2

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

4-(4-Fluorophenyl)-2-oxo-1,2,5,6-tetrahydrobenzo[*h*]quinoline-3- carbonitrile

Crystal data

$C_{20}H_{13}FN_2O$
$M_r = 316.32$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.116\ (10)$ Å
$b = 9.278\ (12)$ Å
$c = 11.263\ (14)$ Å
$\alpha = 98.674\ (19)°$
$\beta = 105.095\ (17)°$
$\gamma = 104.846\ (18)°$
$V = 769.7\ (16)$ Å^3
$Z = 2$
$F(000) = 328$
$D_x = 1.365$ Mg m^{-3}
Melting point > 598 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 929 reflections
$\theta = 2.3–25.4°$
$\mu = 0.09$ mm^{-1}
$T = 298$ K
Block, colourless
0.48 × 0.35 × 0.33 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.956, T_{max} = 0.970
3950 measured reflections
2656 independent reflections
1399 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 25.0°, θ_{min} = 2.3°
$h = -9 \rightarrow 9$
$k = -11 \rightarrow 8$
$l = -9 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.144
S = 1.00
2656 reflections
240 parameters
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
$w = 1/[\sigma^2(F_o^2) + (0.0683P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
F1	0.2899 (2)	0.4261 (2)	−0.18711 (16)	0.1127 (7)	
N1	0.2029 (3)	0.1315 (2)	0.45914 (18)	0.0580 (6)	
H1	0.1926	0.0948	0.5235	0.070*	
N2	−0.2136 (3)	0.1660 (3)	0.0916 (2)	0.0781 (7)	
O1	−0.101 (3)	0.0761 (19)	0.3875 (16)	0.063 (2)	0.489 (17)
O1′	−0.100 (2)	0.0203 (19)	0.3604 (16)	0.063 (2)	0.511 (17)
C1	0.0482 (3)	0.1170 (3)	0.3667 (2)	0.0589 (7)	
C2	0.0742 (3)	0.1847 (3)	0.2646 (2)	0.0474 (6)	
C3	0.2423 (3)	0.2493 (3)	0.2576 (2)	0.0449 (6)	
C4	0.3947 (3)	0.2594 (3)	0.3564 (2)	0.0514 (7)	
C5	0.3716 (3)	0.1991 (3)	0.4576 (2)	0.0441 (6)	
C6	0.5250 (3)	0.2014 (3)	0.5626 (2)	0.0472 (6)	
C7	0.5053 (4)	0.1393 (3)	0.6645 (2)	0.0611 (7)	
H7	0.3908	0.0975	0.6694	0.073*	
C8	0.6514 (4)	0.1387 (3)	0.7579 (2)	0.0673 (8)	
H8	0.6354	0.0973	0.8259	0.081*	
C9	0.8191 (4)	0.1978 (3)	0.7521 (3)	0.0705 (8)	

H9	0.9181	0.1954	0.8149	0.085*	
C10	0.8420 (4)	0.2613 (4)	0.6529 (3)	0.0817 (9)	
H10	0.9575	0.3021	0.6496	0.098*	
C11	0.6977 (4)	0.2660 (3)	0.5580 (2)	0.0652 (8)	
C12	0.7151 (13)	0.2943 (16)	0.4310 (10)	0.060 (2)	0.435 (13)
H12A	0.8345	0.3611	0.4429	0.072*	0.435 (13)
H12B	0.6964	0.1979	0.3740	0.072*	0.435 (13)
C13	0.5770 (13)	0.3675 (14)	0.3755 (13)	0.061 (3)	0.435 (13)
H13A	0.5955	0.4640	0.4323	0.073*	0.435 (13)
H13B	0.5872	0.3880	0.2953	0.073*	0.435 (13)
C12′	0.7237 (10)	0.3759 (13)	0.4687 (7)	0.069 (2)	0.565 (13)
H12C	0.7097	0.4729	0.5027	0.083*	0.565 (13)
H12D	0.8432	0.3954	0.4608	0.083*	0.565 (13)
C13′	0.5852 (10)	0.3014 (12)	0.3417 (7)	0.059 (2)	0.565 (13)
H13C	0.6068	0.2095	0.3046	0.071*	0.565 (13)
H13D	0.5936	0.3710	0.2858	0.071*	0.565 (13)
C14	0.2601 (3)	0.3026 (3)	0.1417 (2)	0.0493 (6)	
C15	0.2276 (4)	0.4341 (3)	0.1176 (3)	0.0681 (8)	
H15	0.1976	0.4956	0.1764	0.082*	
C16	0.2388 (4)	0.4774 (4)	0.0065 (3)	0.0769 (9)	
H16	0.2165	0.5671	−0.0098	0.092*	
C17	0.2827 (4)	0.3865 (4)	−0.0771 (3)	0.0729 (9)	
C18	0.3162 (4)	0.2565 (4)	−0.0566 (3)	0.0858 (10)	
H18	0.3456	0.1957	−0.1163	0.103*	
C19	0.3064 (4)	0.2146 (4)	0.0539 (3)	0.0769 (9)	
H19	0.3314	0.1256	0.0696	0.092*	
C20	−0.0853 (4)	0.1739 (3)	0.1674 (2)	0.0561 (7)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0932 (13)	0.1675 (19)	0.0723 (12)	0.0028 (12)	0.0250 (10)	0.0801 (12)
N1	0.0489 (13)	0.0912 (17)	0.0447 (12)	0.0206 (12)	0.0199 (11)	0.0405 (12)
N2	0.0698 (17)	0.100 (2)	0.0663 (16)	0.0261 (15)	0.0106 (14)	0.0435 (15)
O1	0.0480 (12)	0.100 (8)	0.058 (6)	0.025 (5)	0.027 (3)	0.044 (5)
O1′	0.0480 (12)	0.100 (8)	0.058 (6)	0.025 (5)	0.027 (3)	0.044 (5)
C1	0.0495 (16)	0.088 (2)	0.0505 (16)	0.0231 (15)	0.0207 (14)	0.0367 (15)
C2	0.0511 (15)	0.0574 (16)	0.0420 (14)	0.0187 (13)	0.0187 (12)	0.0256 (12)
C3	0.0535 (15)	0.0467 (15)	0.0418 (14)	0.0153 (12)	0.0212 (12)	0.0207 (12)
C4	0.0509 (15)	0.0569 (16)	0.0503 (15)	0.0113 (13)	0.0198 (13)	0.0266 (13)
C5	0.0461 (14)	0.0482 (15)	0.0414 (14)	0.0141 (12)	0.0164 (12)	0.0163 (12)
C6	0.0485 (15)	0.0505 (16)	0.0426 (14)	0.0140 (13)	0.0143 (12)	0.0131 (12)
C7	0.0549 (17)	0.078 (2)	0.0479 (16)	0.0119 (14)	0.0124 (13)	0.0282 (14)
C8	0.072 (2)	0.068 (2)	0.0521 (17)	0.0144 (16)	0.0056 (16)	0.0245 (15)
C9	0.064 (2)	0.080 (2)	0.0585 (19)	0.0225 (17)	0.0024 (15)	0.0179 (16)
C10	0.0517 (18)	0.114 (3)	0.080 (2)	0.0235 (18)	0.0158 (16)	0.037 (2)
C11	0.0536 (17)	0.085 (2)	0.0588 (17)	0.0193 (15)	0.0158 (14)	0.0276 (16)
C12	0.043 (4)	0.072 (6)	0.068 (5)	0.015 (5)	0.020 (4)	0.026 (4)

C13	0.065 (5)	0.062 (6)	0.057 (5)	0.012 (4)	0.024 (4)	0.024 (4)
C12′	0.055 (3)	0.079 (5)	0.071 (4)	0.010 (4)	0.021 (3)	0.029 (4)
C13′	0.049 (3)	0.071 (5)	0.062 (5)	0.010 (4)	0.024 (3)	0.032 (4)
C14	0.0499 (15)	0.0571 (16)	0.0440 (15)	0.0110 (13)	0.0178 (12)	0.0253 (13)
C15	0.084 (2)	0.0655 (19)	0.0653 (19)	0.0249 (16)	0.0280 (16)	0.0360 (15)
C16	0.077 (2)	0.075 (2)	0.079 (2)	0.0134 (17)	0.0159 (18)	0.0533 (18)
C17	0.0537 (18)	0.108 (3)	0.0502 (18)	−0.0009 (18)	0.0128 (14)	0.0486 (19)
C18	0.104 (3)	0.112 (3)	0.064 (2)	0.038 (2)	0.0474 (19)	0.041 (2)
C19	0.112 (3)	0.086 (2)	0.0628 (19)	0.046 (2)	0.0480 (19)	0.0436 (17)
C20	0.0602 (18)	0.0676 (18)	0.0495 (17)	0.0195 (15)	0.0222 (15)	0.0318 (14)

Geometric parameters (Å, º)

F1—C17	1.356 (3)	C10—C11	1.381 (4)
N1—C5	1.358 (3)	C10—H10	0.9300
N1—C1	1.367 (3)	C11—C12	1.528 (9)
N1—H1	0.8600	C11—C12′	1.550 (8)
N2—C20	1.139 (3)	C12—C13	1.505 (14)
O1—C1	1.267 (18)	C12—H12A	0.9700
O1′—C1	1.279 (18)	C12—H12B	0.9700
C1—C2	1.428 (3)	C13—H13A	0.9700
C2—C3	1.370 (3)	C13—H13B	0.9700
C2—C20	1.431 (4)	C12′—C13′	1.501 (12)
C3—C4	1.404 (3)	C12′—H12C	0.9700
C3—C14	1.491 (3)	C12′—H12D	0.9700
C4—C5	1.377 (3)	C13′—H13C	0.9700
C4—C13	1.499 (10)	C13′—H13D	0.9700
C4—C13′	1.553 (8)	C14—C15	1.363 (4)
C5—C6	1.470 (3)	C14—C19	1.376 (4)
C6—C7	1.387 (3)	C15—C16	1.389 (4)
C6—C11	1.394 (4)	C15—H15	0.9300
C7—C8	1.367 (4)	C16—C17	1.347 (4)
C7—H7	0.9300	C16—H16	0.9300
C8—C9	1.354 (4)	C17—C18	1.342 (4)
C8—H8	0.9300	C18—C19	1.375 (4)
C9—C10	1.371 (4)	C18—H18	0.9300
C9—H9	0.9300	C19—H19	0.9300
C5—N1—C1	125.3 (2)	C13—C12—H12A	109.9
C5—N1—H1	117.4	C11—C12—H12A	109.9
C1—N1—H1	117.4	C13—C12—H12B	109.9
O1—C1—N1	119.7 (9)	C11—C12—H12B	109.9
O1′—C1—N1	120.2 (8)	H12A—C12—H12B	108.3
O1—C1—C2	124.0 (9)	C4—C13—C12	108.2 (9)
O1′—C1—C2	123.2 (8)	C4—C13—H13A	110.1
N1—C1—C2	114.7 (2)	C12—C13—H13A	110.1
C3—C2—C1	121.7 (2)	C4—C13—H13B	110.1
C3—C2—C20	122.2 (2)	C12—C13—H13B	110.1

C1—C2—C20	116.0 (2)	H13A—C13—H13B	108.4
C2—C3—C4	120.1 (2)	C13′—C12′—C11	108.2 (7)
C2—C3—C14	119.1 (2)	C13′—C12′—H12C	110.1
C4—C3—C14	120.8 (2)	C11—C12′—H12C	110.1
C5—C4—C3	118.8 (2)	C13′—C12′—H12D	110.1
C5—C4—C13	116.3 (5)	C11—C12′—H12D	110.1
C3—C4—C13	122.8 (5)	H12C—C12′—H12D	108.4
C5—C4—C13′	118.0 (4)	C12′—C13′—C4	109.8 (7)
C3—C4—C13′	121.8 (4)	C12′—C13′—H13C	109.7
N1—C5—C4	119.4 (2)	C4—C13′—H13C	109.7
N1—C5—C6	118.8 (2)	C12′—C13′—H13D	109.7
C4—C5—C6	121.8 (2)	C4—C13′—H13D	109.7
C7—C6—C11	118.7 (2)	H13C—C13′—H13D	108.2
C7—C6—C5	122.9 (2)	C15—C14—C19	118.4 (2)
C11—C6—C5	118.4 (2)	C15—C14—C3	122.3 (2)
C8—C7—C6	121.1 (3)	C19—C14—C3	119.2 (2)
C8—C7—H7	119.5	C14—C15—C16	120.9 (3)
C6—C7—H7	119.5	C14—C15—H15	119.5
C9—C8—C7	120.4 (3)	C16—C15—H15	119.5
C9—C8—H8	119.8	C17—C16—C15	118.4 (3)
C7—C8—H8	119.8	C17—C16—H16	120.8
C8—C9—C10	119.5 (3)	C15—C16—H16	120.8
C8—C9—H9	120.2	C18—C17—C16	122.5 (3)
C10—C9—H9	120.2	C18—C17—F1	118.7 (3)
C9—C10—C11	121.6 (3)	C16—C17—F1	118.8 (3)
C9—C10—H10	119.2	C17—C18—C19	118.9 (3)
C11—C10—H10	119.2	C17—C18—H18	120.5
C10—C11—C6	118.7 (3)	C19—C18—H18	120.5
C10—C11—C12	121.7 (4)	C18—C19—C14	120.9 (3)
C6—C11—C12	117.1 (4)	C18—C19—H19	119.6
C10—C11—C12′	120.9 (4)	C14—C19—H19	119.6
C6—C11—C12′	118.5 (4)	N2—C20—C2	178.8 (3)
C13—C12—C11	108.8 (9)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.86	2.08	2.883 (3)	155
C7—H7···O1^{i}	0.93	2.35	3.223 (3)	157
C12—H12*B*···O1^{ii}	0.97	2.21	2.863 (3)	124
C13—H13*B*···F1^{iii}	0.97	2.42	3.270 (3)	147
C15—H15···*Cg*3^{iv}	0.93	2.90	3.671 (3)	141

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