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4-(3,3-Dimethylperhydro-1,3-oxazolo[3,4-*a*]pyridin-1-yl)-2,8-bis(trifluoromethyl)quinoline

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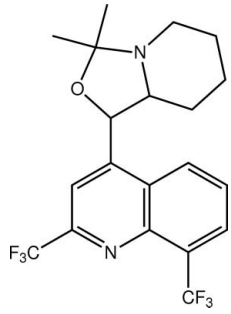
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.002 Å; R factor = 0.047; wR factor = 0.141; data-to-parameter ratio = 16.2.

An L-shaped conformation is found in the title molecule, $C_{20}H_{20}F_6N_2O$, the C—C—C—C torsion angle linking the two fused-ring systems being −92.80 (19)°. The oxazole ring adopts an envelope conformation [the N atom lies 0.579 (2) Å out of the plane defined by the remaining atoms], and the piperidine ring has a chair conformation. Supramolecular chains are found in the crystal structure that are sustained by C—H···π and π–π [3.6089 (10) Å] interactions.

Related literature

For information on mefloquine and its derivatives, see: Maguire *et al.* (2006); Croft & Herxheimer (2002); Lima *et al.* (2002); Biot *et al.* (2000); Roesner *et al.* (1981); Kunin & Ellis (2007). For the synthesis of 1,3-oxazolidines, see: Bergmann *et al.* (1953); Oh *et al.* (2000); Saba *et al.* (2007); Page *et al.* (2007); Kukharev *et al.* (2007); Delgado *et al.* (1987). For the biological activity of 1,3-oxazolidines, see: Moloney *et al.* (1998); Andes *et al.* (2002); Kumar *et al.* (2009).



Experimental

Crystal data

$C_{20}H_{20}F_6N_2O$
M_r = 418.38
Triclinic, $P\overline{1}$
a = 8.4192 (3) Å
b = 9.1833 (4) Å
c = 12.4424 (4) Å
α = 87.912 (2)°
β = 86.666 (2)°
γ = 78.804 (2)°
V = 941.78 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 120 K
0.65 × 0.30 × 0.25 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
T_{min} = 0.643, T_{max} = 0.746
16907 measured reflections
4275 independent reflections
3107 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.141
S = 1.06
4275 reflections
264 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

Cg is the centroid of the C4–C9 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15c···Cg^{i}	0.98	2.87	3.781 (2)	155

Symmetry code: (i) $x-1, y, z$.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: EZ2202).

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supporting information

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4-(3,3-Dimethylperhydro-1,3-oxazolo[3,4-*a*]pyridin-1-yl)-2,8-bis(trifluoromethyl)quinoline

James L. Wardell, Solange M. S. V. Wardell and Edward R. T. Tiekink

S1. Comment

Mefloquine, manufactured as the racemic erythro hydrochloride salt is a synthetic analogue of quinine used in the prevention and treatment for malaria in combination with other drugs (Maguire *et al.*, 2006). However, despite its efficacy, this orally-administered drug possesses several important physical and psychological adverse side-effects, such as birth defects, anxiety, aggression, seizures, nightmares, neuropathy, insomnia, central nervous system problems, acute depression, urinary disorders, *etc*. (Croft & Herxheimer, 2002). Due to these effects, mefloquine analogues have been synthesized with the goals of increasing the efficacy and eliminating adverse side-effects (Lima *et al.*, 2002; Biot *et al.*, 2000; Roesner *et al.*, 1981). Mefloquine derivatives are also undergoing tests against other diseases, for example, as anti-viral and anti-tuberculosis agents (Kunin & Ellis, 2007). In the quest for new derivatives, the title compound, 5-[2,8-bis-(trifluoromethyl)quinolin-4-yl)-hexahydro-3*H*-oxazolo[3,4-a]pyridine-2-oxaindolizidine (I) has been obtained.

Oxazolidines are frequently prepared from 2-amino-1-hydroxyalkanes and carbonyl compounds (Bergmann *et al.*, 1953; Oh *et al.*, 2000; Saba *et al.*, 2007; Page *et al.*, 2007); in particular cases, azeotropic removal of water or the use of a catalyst is involved (Page *et al.*, 2007). However, problems of stability of oxazolidines and formation of tautomeric mixtures of the oxazolidines and the corresponding imines can limit or complicate this synthetic route (Page *et al.*, 2007). Alternative routes to hexahydro-3*H*-oxazolo[3,4-a]pyridine derivatives include the $Hg(OAc)_2$ catalysed cyclization of 2-(vinyloxymethyl)piperidine (Kukharev *et al.*, 2007) and use of 1-naphthalenyl 2-pyridinyl ketone (Delgado *et al.*, 1987). 1,3-Oxazolidine derivatives, in general, have been shown to have useful biological activities (Moloney *et al.*, 1998; Andes *et al.*, 2002; Kumar *et al.*, 2009). The title compound, (I), was isolated unexpectedly from a solution of mefloquine hydrochloride and 2-hydroxybenzoic acid in acetone, followed by initial by recrystallisation from iso-propanol, and finally from EtOH.

The molecular structure of (I), Fig. 1, adopts an L-shaped conformation with the quinoline group being approximately orthogonal to the rest of the molecule; for example, the C2–C3–C12–C16 torsion angle is -92.80 (19) °. The five-membered oxazole ring adopts an envelope conformation with the N2 atom lying 0.579 (2) Å out of the plane defined by the remaining atoms. The piperidine ring adopts a chair conformation. The presence of C–H···π, Table 1, and π–π [ring centroid(C4–C9)···ring centroid(C4–C9)^{i} distance = 3.6089 (10) Å for *i*: 1-*x*, 1-*y*, 2-*z*] interactions feature in the crystal packing. Thus, centrosymmetrically related molecules are connected via π–π interactions, and these are linked into a supramolecular chain via C–H···π contacts, Fig. 2.

S2. Experimental

A mixture of racemic erythro mefloquinium chloride (1 mmol) and 2-hydroxybenzoic acid (1 mmol) in acetone (20 ml) was refluxed for 3 h. The reaction mixture was rotary evaporated and the residue was taken up in isopropanol. Two crops of crystals were collected on maintaining the solution at room temperature. From the second crop, on recrystallisation

from EtOH, a small amount of the title compound was obtained, m.p. 424–426 K.

S3. Refinement

The C-bound H atoms were geometrically placed (C–H = 0.95–1.00 Å) and refined as riding with U_{iso}(H) = 1.2-1.5U_{eq}(C).

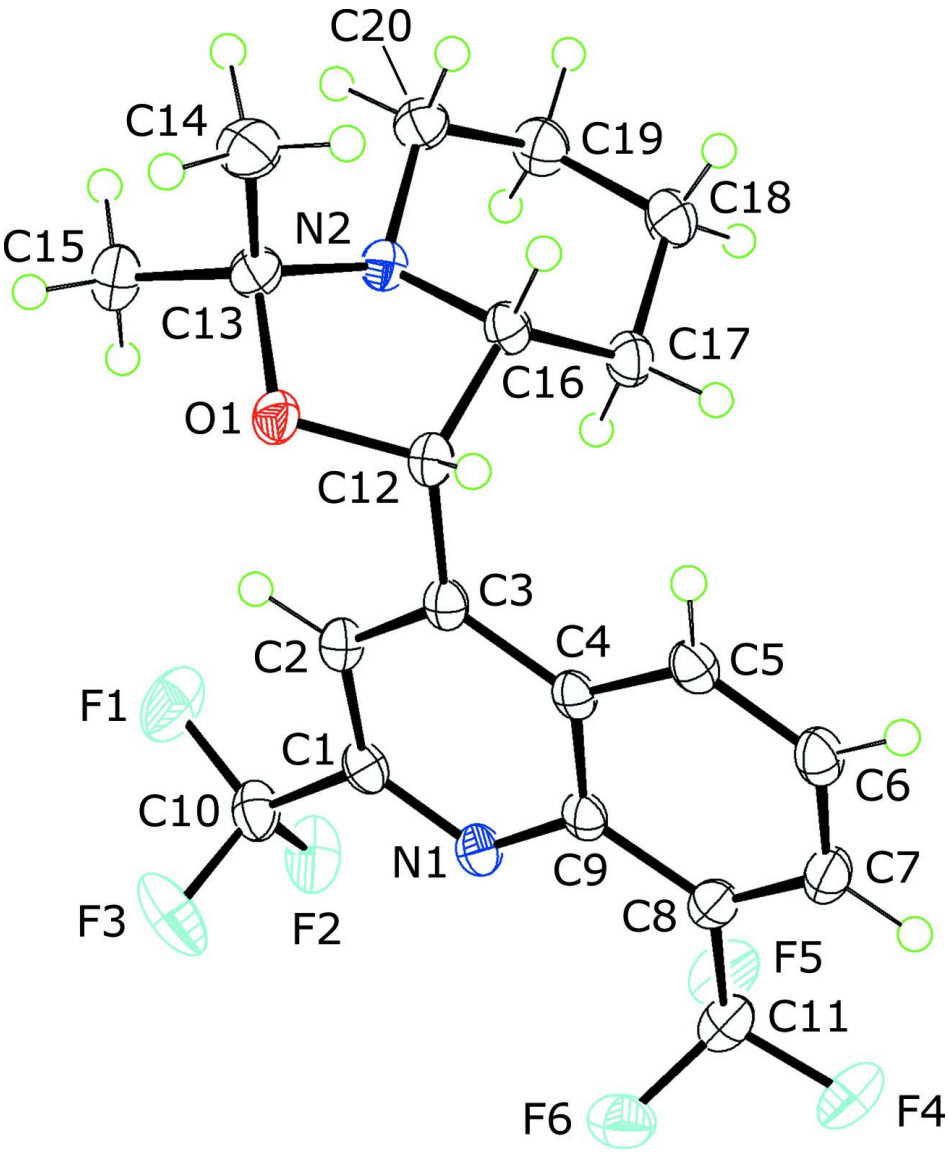

Figure 1

The molecular structure of (I) showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level.

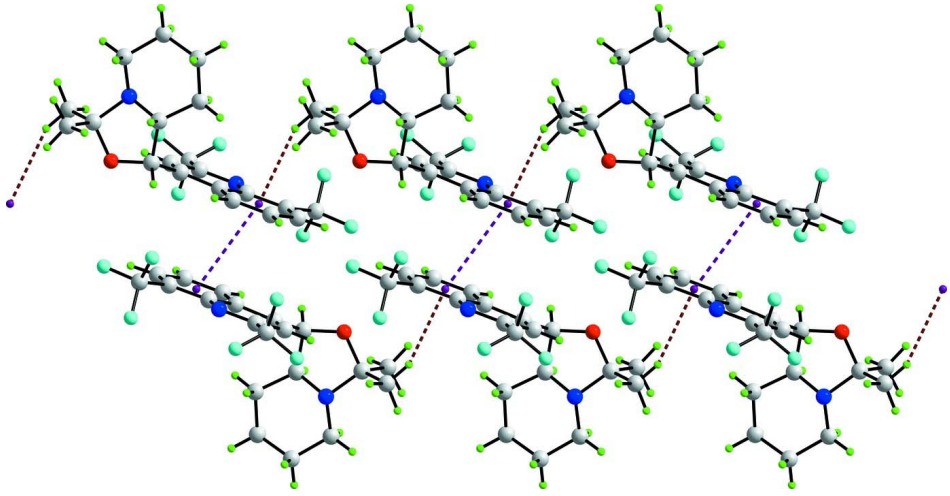

Figure 2

A view of a supramolecular chain in (I) aligned along the *a* axis. The C–H···π and π–π interactions are shown as brown and purple dashed lines, respectively. Colour code: F, cyan; O, red; N, blue; C, grey; and H, green.

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Crystal data

$C_{20}H_{20}F_6N_2O$
$M_r = 418.38$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.4192$ (3) Å
$b = 9.1833$ (4) Å
$c = 12.4424$ (4) Å
$\alpha = 87.912$ (2)°
$\beta = 86.666$ (2)°
$\gamma = 78.804$ (2)°
$V = 941.78$ (6) Å^3
$Z = 2$
$F(000) = 432$
$D_x = 1.475$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 12184 reflections
$\theta = 2.9$–27.5°
$\mu = 0.13$ mm^{-1}
$T = 120$ K
Block, colourless
0.65 × 0.30 × 0.25 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Radiation source: Enraf Nonius FR591 rotating anode
10 cm confocal mirrors monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
$T_{min} = 0.643$, $T_{max} = 0.746$
16907 measured reflections
4275 independent reflections
3107 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 27.4°$, $\theta_{min} = 3.0°$
$h = -10 \rightarrow 10$
$k = -11 \rightarrow 11$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.141$
$S = 1.06$
4275 reflections
264 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0739P)^2 + 0.249P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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}
F1	0.24470 (15)	0.13631 (13)	0.70186 (12)	0.0465 (4)
F2	0.48941 (14)	0.02882 (12)	0.72734 (10)	0.0376 (3)
F3	0.31274 (17)	0.05404 (14)	0.85902 (11)	0.0489 (4)
F4	1.00086 (13)	0.26530 (14)	0.94688 (10)	0.0398 (3)
F5	0.90320 (13)	0.18513 (14)	0.80980 (9)	0.0369 (3)
F6	0.80523 (14)	0.14596 (13)	0.96979 (9)	0.0357 (3)
O1	0.04978 (14)	0.65337 (14)	0.77211 (9)	0.0225 (3)
N1	0.54732 (17)	0.26383 (16)	0.83292 (11)	0.0209 (3)
N2	0.13591 (17)	0.69425 (16)	0.59985 (11)	0.0208 (3)
C1	0.4030 (2)	0.27072 (19)	0.79573 (13)	0.0205 (4)
C2	0.2882 (2)	0.40134 (19)	0.77803 (13)	0.0208 (4)
H2	0.1866	0.3973	0.7501	0.025*
C3	0.3263 (2)	0.53470 (19)	0.80200 (13)	0.0190 (4)
C4	0.4797 (2)	0.53404 (19)	0.84578 (13)	0.0183 (4)
C5	0.5296 (2)	0.6653 (2)	0.87684 (13)	0.0221 (4)
H5	0.4579	0.7585	0.8709	0.027*
C6	0.6799 (2)	0.6584 (2)	0.91518 (14)	0.0248 (4)
H6	0.7114	0.7467	0.9360	0.030*
C7	0.7882 (2)	0.5216 (2)	0.92398 (14)	0.0258 (4)
H7	0.8934	0.5188	0.9488	0.031*
C8	0.7437 (2)	0.3925 (2)	0.89724 (13)	0.0222 (4)
C9	0.5868 (2)	0.3955 (2)	0.85806 (13)	0.0195 (4)
C10	0.3631 (2)	0.1221 (2)	0.77122 (16)	0.0273 (4)
C11	0.8617 (2)	0.2472 (2)	0.90593 (15)	0.0280 (4)
C12	0.2119 (2)	0.67903 (19)	0.77676 (14)	0.0200 (4)
H12	0.2150	0.7518	0.8341	0.024*
C13	−0.0137 (2)	0.7020 (2)	0.66828 (14)	0.0225 (4)
C14	−0.1190 (2)	0.8573 (2)	0.67829 (16)	0.0313 (5)
H14A	−0.2044	0.8555	0.7351	0.047*
H14B	−0.1685	0.8881	0.6097	0.047*
H14C	−0.0516	0.9277	0.6966	0.047*
C15	−0.1106 (2)	0.5903 (2)	0.63459 (16)	0.0301 (4)

H15A	−0.0419	0.4911	0.6343	0.045*
H15B	−0.1486	0.6169	0.5622	0.045*
H15C	−0.2040	0.5908	0.6854	0.045*
C16	0.2497 (2)	0.7487 (2)	0.66532 (13)	0.0211 (4)
H16	0.2174	0.8591	0.6692	0.025*
C17	0.4194 (2)	0.7103 (2)	0.61295 (14)	0.0248 (4)
H17A	0.4541	0.6012	0.6094	0.030*
H17B	0.4965	0.7488	0.6563	0.030*
C18	0.4196 (2)	0.7800 (2)	0.49901 (15)	0.0290 (4)
H18A	0.4013	0.8895	0.5037	0.035*
H18B	0.5269	0.7463	0.4617	0.035*
C19	0.2881 (2)	0.7372 (2)	0.43406 (15)	0.0289 (4)
H19A	0.2825	0.7929	0.3643	0.035*
H19B	0.3165	0.6299	0.4189	0.035*
C20	0.1239 (2)	0.7705 (2)	0.49433 (14)	0.0251 (4)
H20A	0.0896	0.8789	0.5035	0.030*
H20B	0.0420	0.7359	0.4529	0.030*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0385 (7)	0.0273 (7)	0.0775 (10)	−0.0082 (5)	−0.0226 (7)	−0.0122 (6)
F2	0.0292 (6)	0.0254 (6)	0.0579 (8)	−0.0043 (5)	0.0073 (5)	−0.0162 (6)
F3	0.0677 (9)	0.0281 (7)	0.0531 (8)	−0.0219 (6)	0.0212 (7)	−0.0005 (6)
F4	0.0252 (6)	0.0483 (8)	0.0446 (7)	0.0006 (5)	−0.0134 (5)	−0.0066 (6)
F5	0.0292 (6)	0.0482 (8)	0.0290 (6)	0.0045 (5)	0.0007 (5)	−0.0115 (5)
F6	0.0369 (7)	0.0323 (7)	0.0348 (6)	−0.0004 (5)	−0.0030 (5)	0.0063 (5)
O1	0.0172 (6)	0.0279 (7)	0.0225 (6)	−0.0056 (5)	0.0007 (5)	0.0008 (5)
N1	0.0202 (7)	0.0227 (8)	0.0199 (7)	−0.0050 (6)	0.0032 (6)	−0.0019 (6)
N2	0.0192 (7)	0.0215 (8)	0.0218 (7)	−0.0043 (6)	−0.0002 (6)	−0.0016 (6)
C1	0.0232 (9)	0.0188 (9)	0.0199 (8)	−0.0063 (7)	0.0041 (7)	−0.0024 (7)
C2	0.0189 (8)	0.0233 (9)	0.0213 (9)	−0.0065 (7)	0.0010 (7)	−0.0026 (7)
C3	0.0192 (8)	0.0228 (9)	0.0158 (8)	−0.0065 (7)	0.0025 (6)	−0.0026 (7)
C4	0.0200 (8)	0.0214 (9)	0.0142 (8)	−0.0068 (7)	0.0026 (6)	−0.0007 (7)
C5	0.0256 (9)	0.0227 (9)	0.0192 (8)	−0.0084 (7)	0.0014 (7)	0.0001 (7)
C6	0.0287 (10)	0.0292 (10)	0.0199 (9)	−0.0138 (8)	−0.0012 (7)	−0.0020 (7)
C7	0.0212 (9)	0.0377 (11)	0.0208 (9)	−0.0109 (8)	−0.0023 (7)	−0.0008 (8)
C8	0.0189 (8)	0.0319 (10)	0.0154 (8)	−0.0048 (7)	0.0011 (6)	0.0002 (7)
C9	0.0211 (8)	0.0247 (9)	0.0138 (8)	−0.0080 (7)	0.0023 (6)	0.0004 (7)
C10	0.0231 (9)	0.0216 (9)	0.0373 (11)	−0.0057 (7)	0.0032 (8)	−0.0038 (8)
C11	0.0220 (9)	0.0368 (11)	0.0244 (10)	−0.0030 (8)	−0.0026 (7)	−0.0046 (8)
C12	0.0186 (8)	0.0210 (9)	0.0213 (9)	−0.0056 (7)	−0.0002 (6)	−0.0032 (7)
C13	0.0208 (9)	0.0229 (9)	0.0230 (9)	−0.0021 (7)	−0.0011 (7)	−0.0013 (7)
C14	0.0270 (10)	0.0282 (11)	0.0354 (11)	0.0014 (8)	0.0035 (8)	0.0004 (8)
C15	0.0240 (10)	0.0369 (11)	0.0315 (10)	−0.0111 (8)	−0.0004 (8)	−0.0041 (9)
C16	0.0230 (9)	0.0202 (9)	0.0214 (9)	−0.0075 (7)	−0.0008 (7)	−0.0018 (7)
C17	0.0216 (9)	0.0297 (10)	0.0242 (9)	−0.0085 (8)	0.0005 (7)	0.0006 (8)
C18	0.0262 (10)	0.0349 (11)	0.0264 (10)	−0.0093 (8)	0.0039 (7)	0.0030 (8)

C19	0.0301 (10)	0.0345 (11)	0.0223 (9)	−0.0077 (8)	0.0025 (7)	−0.0009 (8)
C20	0.0257 (9)	0.0267 (10)	0.0227 (9)	−0.0041 (8)	−0.0025 (7)	−0.0005 (7)

Geometric parameters (Å, º)

F1—C10	1.341 (2)	C7—H7	0.9500
F2—C10	1.333 (2)	C8—C9	1.429 (2)
F3—C10	1.328 (2)	C8—C11	1.506 (3)
F4—C11	1.346 (2)	C12—C16	1.548 (2)
F5—C11	1.342 (2)	C12—H12	1.0000
F6—C11	1.340 (2)	C13—C15	1.513 (3)
O1—C12	1.434 (2)	C13—C14	1.531 (3)
O1—C13	1.449 (2)	C14—H14A	0.9800
N1—C1	1.315 (2)	C14—H14B	0.9800
N1—C9	1.366 (2)	C14—H14C	0.9800
N2—C16	1.462 (2)	C15—H15A	0.9800
N2—C20	1.465 (2)	C15—H15B	0.9800
N2—C13	1.470 (2)	C15—H15C	0.9800
C1—C2	1.406 (2)	C16—C17	1.518 (2)
C1—C10	1.513 (2)	C16—H16	1.0000
C2—C3	1.372 (2)	C17—C18	1.534 (3)
C2—H2	0.9500	C17—H17A	0.9900
C3—C4	1.429 (2)	C17—H17B	0.9900
C3—C12	1.514 (2)	C18—C19	1.527 (3)
C4—C9	1.419 (2)	C18—H18A	0.9900
C4—C5	1.424 (2)	C18—H18B	0.9900
C5—C6	1.367 (3)	C19—C20	1.516 (3)
C5—H5	0.9500	C19—H19A	0.9900
C6—C7	1.407 (3)	C19—H19B	0.9900
C6—H6	0.9500	C20—H20A	0.9900
C7—C8	1.368 (3)	C20—H20B	0.9900
C12—O1—C13	110.26 (13)	C16—C12—H12	109.4
C1—N1—C9	116.60 (15)	O1—C13—N2	101.73 (13)
C16—N2—C20	111.29 (14)	O1—C13—C15	107.83 (15)
C16—N2—C13	105.69 (13)	N2—C13—C15	110.94 (14)
C20—N2—C13	117.78 (14)	O1—C13—C14	109.00 (14)
N1—C1—C2	125.68 (16)	N2—C13—C14	115.09 (15)
N1—C1—C10	114.78 (16)	C15—C13—C14	111.56 (15)
C2—C1—C10	119.54 (15)	C13—C14—H14A	109.5
C3—C2—C1	118.53 (16)	C13—C14—H14B	109.5
C3—C2—H2	120.7	H14A—C14—H14B	109.5
C1—C2—H2	120.7	C13—C14—H14C	109.5
C2—C3—C4	118.39 (16)	H14A—C14—H14C	109.5
C2—C3—C12	120.45 (15)	H14B—C14—H14C	109.5
C4—C3—C12	121.08 (15)	C13—C15—H15A	109.5
C9—C4—C5	118.85 (15)	C13—C15—H15B	109.5
C9—C4—C3	117.96 (15)	H15A—C15—H15B	109.5

C5—C4—C3	123.19 (16)	C13—C15—H15C	109.5
C6—C5—C4	120.61 (17)	H15A—C15—H15C	109.5
C6—C5—H5	119.7	H15B—C15—H15C	109.5
C4—C5—H5	119.7	N2—C16—C17	109.60 (14)
C5—C6—C7	120.52 (17)	N2—C16—C12	100.79 (13)
C5—C6—H6	119.7	C17—C16—C12	119.71 (15)
C7—C6—H6	119.7	N2—C16—H16	108.7
C8—C7—C6	120.74 (16)	C17—C16—H16	108.7
C8—C7—H7	119.6	C12—C16—H16	108.7
C6—C7—H7	119.6	C16—C17—C18	109.14 (15)
C7—C8—C9	120.17 (17)	C16—C17—H17A	109.9
C7—C8—C11	120.07 (16)	C18—C17—H17A	109.9
C9—C8—C11	119.74 (16)	C16—C17—H17B	109.9
N1—C9—C4	122.79 (15)	C18—C17—H17B	109.9
N1—C9—C8	118.15 (16)	H17A—C17—H17B	108.3
C4—C9—C8	119.06 (16)	C19—C18—C17	111.21 (15)
F3—C10—F2	106.77 (16)	C19—C18—H18A	109.4
F3—C10—F1	106.58 (16)	C17—C18—H18A	109.4
F2—C10—F1	106.43 (15)	C19—C18—H18B	109.4
F3—C10—C1	112.06 (16)	C17—C18—H18B	109.4
F2—C10—C1	112.82 (15)	H18A—C18—H18B	108.0
F1—C10—C1	111.76 (16)	C20—C19—C18	111.32 (15)
F6—C11—F5	106.96 (16)	C20—C19—H19A	109.4
F6—C11—F4	106.30 (15)	C18—C19—H19A	109.4
F5—C11—F4	106.15 (14)	C20—C19—H19B	109.4
F6—C11—C8	113.30 (14)	C18—C19—H19B	109.4
F5—C11—C8	112.29 (15)	H19A—C19—H19B	108.0
F4—C11—C8	111.37 (16)	N2—C20—C19	108.88 (15)
O1—C12—C3	109.96 (14)	N2—C20—H20A	109.9
O1—C12—C16	104.86 (13)	C19—C20—H20A	109.9
C3—C12—C16	113.55 (14)	N2—C20—H20B	109.9
O1—C12—H12	109.4	C19—C20—H20B	109.9
C3—C12—H12	109.4	H20A—C20—H20B	108.3

C9—N1—C1—C2	1.2 (3)	C7—C8—C11—F5	−115.48 (18)
C9—N1—C1—C10	−178.76 (14)	C9—C8—C11—F5	62.7 (2)
N1—C1—C2—C3	−0.7 (3)	C7—C8—C11—F4	3.4 (2)
C10—C1—C2—C3	179.25 (16)	C9—C8—C11—F4	−178.36 (15)
C1—C2—C3—C4	−1.2 (2)	C13—O1—C12—C3	−122.74 (14)
C1—C2—C3—C12	175.52 (14)	C13—O1—C12—C16	−0.32 (17)
C2—C3—C4—C9	2.4 (2)	C2—C3—C12—O1	24.3 (2)
C12—C3—C4—C9	−174.25 (14)	C4—C3—C12—O1	−159.06 (14)
C2—C3—C4—C5	−177.91 (15)	C2—C3—C12—C16	−92.80 (19)
C12—C3—C4—C5	5.4 (2)	C4—C3—C12—C16	83.81 (18)
C9—C4—C5—C6	1.7 (2)	C12—O1—C13—N2	23.98 (16)
C3—C4—C5—C6	−177.97 (16)	C12—O1—C13—C15	140.73 (14)
C4—C5—C6—C7	0.4 (3)	C12—O1—C13—C14	−98.00 (16)
C5—C6—C7—C8	−1.8 (3)	C16—N2—C13—O1	−39.80 (16)

C6—C7—C8—C9	1.1 (3)	C20—N2—C13—O1	−164.85 (14)
C6—C7—C8—C11	179.30 (16)	C16—N2—C13—C15	−154.28 (15)
C1—N1—C9—C4	0.2 (2)	C20—N2—C13—C15	80.67 (19)
C1—N1—C9—C8	−179.11 (15)	C16—N2—C13—C14	77.87 (18)
C5—C4—C9—N1	178.31 (15)	C20—N2—C13—C14	−47.2 (2)
C3—C4—C9—N1	−2.0 (2)	C20—N2—C16—C17	−64.79 (18)
C5—C4—C9—C8	−2.4 (2)	C13—N2—C16—C17	166.23 (14)
C3—C4—C9—C8	177.30 (14)	C20—N2—C16—C12	168.10 (13)
C7—C8—C9—N1	−179.65 (15)	C13—N2—C16—C12	39.12 (16)
C11—C8—C9—N1	2.1 (2)	O1—C12—C16—N2	−23.53 (16)
C7—C8—C9—C4	1.0 (2)	C3—C12—C16—N2	96.54 (15)
C11—C8—C9—C4	−177.20 (14)	O1—C12—C16—C17	−143.66 (15)
N1—C1—C10—F3	81.59 (19)	C3—C12—C16—C17	−23.6 (2)
C2—C1—C10—F3	−98.4 (2)	N2—C16—C17—C18	58.38 (19)
N1—C1—C10—F2	−39.0 (2)	C12—C16—C17—C18	173.97 (15)
C2—C1—C10—F2	141.05 (17)	C16—C17—C18—C19	−52.9 (2)
N1—C1—C10—F1	−158.85 (15)	C17—C18—C19—C20	52.4 (2)
C2—C1—C10—F1	21.2 (2)	C16—N2—C20—C19	62.59 (18)
C7—C8—C11—F6	123.21 (18)	C13—N2—C20—C19	−175.18 (15)
C9—C8—C11—F6	−58.6 (2)	C18—C19—C20—N2	−55.9 (2)

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the C4–C9 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15c···*Cg*^{i}	0.98	2.87	3.781 (2)	155

Symmetry code: (i) *x*−1, *y*, *z*.