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N-[(1*R*,2*S*)-1-(4-Bromophenyl)-2-fluoro-3-(2-methylphenyl)-3-oxopropyl]-4-nitrobenzamide

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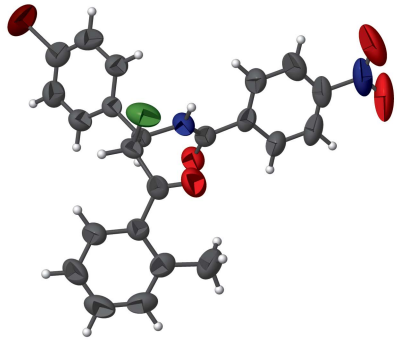
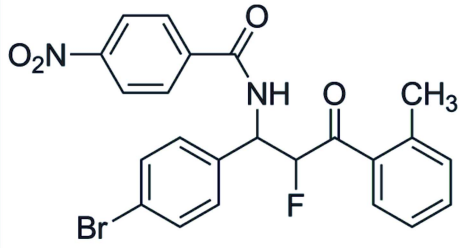
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{23}H_{18}BrFN_2O_4$, contains two chiral carbon centres and the absolute configuration has been confirmed as (1*R*,2*S*). The dihedral angles between the three phenyl rings are 12.4 (4), 34.2 (4) and 44.5 (4)°. In the crystal, molecules are linked by N—H···O hydrogen bonds into chains, which which are further connected by C—H···O interactions, generating a three dimensional network structure.

3D view



Chemical scheme



Structure description

Fluorine is highly important in medicinal chemistry (Wang *et al.*, 2014). The introduction of fluorine into a bioactive molecule often improves the binding affinity, metabolic stability, and bioavailability (Purser *et al.*, 2008). In this context, the *β*-fluoroamine motif is an important structural motif and has been found in a number of drug candidates (Murray *et al.*, 2003; Li *et al.*, 2016). It is generally believed that a *β*-fluoro substitution lowers the pK_a value of the neighboring amines, and can thus modulate many pharmacological properties (Morgenthaler *et al.*, 2007).

In the title compound (Fig. 1), the fluoro and amino substituents adopt an *anti* configuration and the absolute configuration of the two chiral carbon centres, C8 and C9, has been determined as (1*R*,2*S*). In the crystal, molecules are linked by classical N—H···O hydrogen bonds (Table 1, Fig. 2) into [001] chains, which which are further connected by C—H···O interactions, generating a three-dimensional network structure.

Synthesis and crystallization

Sodium bis(trimethylsilyl)amide (NaHMDS, 1.5 ml, 1.0 mol/l in THF) was added to a solution of 2-fluoro-1-(*o*-tolyl)ethan-1-one (228 mg, 1.5 mmol), (*RS*)-*N*-(4-bromobenzylidene)-2-methylpropane-2-sulfinamide (288 mg, 1.0 mmol) and Et_2O (4 ml) at

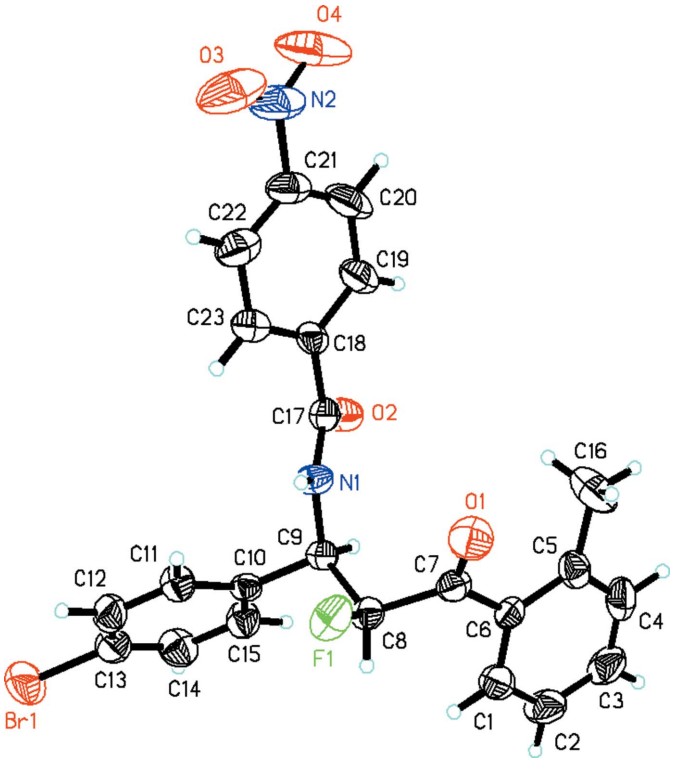


Figure 1
Molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

203 K. The reaction mixture was stirred for 30 min, followed by a routine work-up to give the crude condensation intermediate. Without further purification, the crude intermediate was dissolved in 5 mL HCl/MeOH (4 mol l^{-1}) at room temperature and the mixture was stirred for 20 min. The volatile materials were removed under vacuum, followed by the addition of 4-nitrobenzoyl chloride (184 mg, 1.0 mmol), NEt_3 (202 mg, 2.0 mmol) and THF (3.0 mL). After 3 h, H_2O (5 ml) was added, and the quenched reaction mixture was extracted with ethyl acetate (3 × 20 mL). The combined organic layers were dried over anhydrous Na_2SO_4. Evaporation of the solvent under vacuum was followed by flash chromatography to give the title compound (218 mg, 45%). The resulting compound was recrystallized from ethyl acetate/hexane (1:2) to give colourless crystals.

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.33 (*d*, *J* = 8.0 Hz, 2H), 7.95 (*d*, *J* = 8.0 Hz, 2H), 7.48–7.54 (*m*, 4H), 7.28–7.34 (*m*, 4H), 7.21 (*d*, *J* = 8.0 Hz, 1H), 5.88 (*dd*, *J* = 48.0, 4.0 Hz, 1H), 5.74 (*dd*, *J* = 24.0, 8.0 Hz, 1H), 2.38 (*s*, 3H).

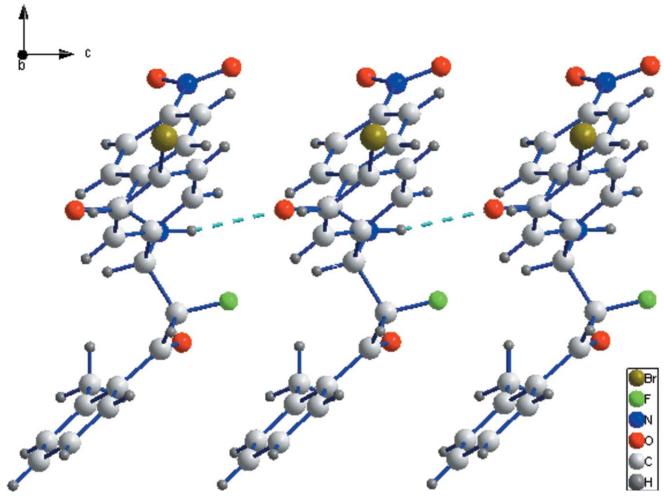


Figure 2
Intermolecular N—H···O interactions in the title compound, shown as dashed lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···F1	0.86 (8)	2.36 (6)	2.728 (9)	106 (5)
N1—H1*A*···O2^{i}	0.86 (8)	2.42 (8)	3.263 (10)	166 (4)
C9—H9···F1^{ii}	0.98	2.39	3.364 (8)	175
C8—H8···O4^{iii}	0.98	2.50	3.387 (12)	150
C9—H9···O2	0.98	2.37	2.758 (9)	103

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{23}H_{18}BrFN_2O_4$
M_r	485.30
Crystal system, space group	Orthorhombic, $P2_12_12$
Temperature (K)	293
a, *b*, *c* (Å)	18.883 (3), 21.006 (3), 5.3312 (8)
V (Å^3)	2114.6 (5)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	1.99
Crystal size (mm)	0.22 × 0.14 × 0.10
Data collection	
Diffractometer	Bruker SMART CCD area detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2007)
T_{min}, T_{max}	0.528, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	17885, 3736, 2701
R_{int}	0.048
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.064, 0.150, 1.13
No. of reflections	3736
No. of parameters	285
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.33, −0.36
Absolute structure	Flack *x* determined using 848 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.008 (19)

Computer programs: *SMART* and *SAINT* (Bruker, 2007), *SHELXTL* (Sheldrick, 2008) and *SHELXL2013* (Sheldrick, 2015).

Refinement

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

Funding information

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full crystallographic data

IUCrData (2018). **3**, x180459 [https://doi.org/10.1107/S2414314618004595]

N-[(1*R*,2*S*)-1-(4-Bromophenyl)-2-fluoro-3-(2-methylphenyl)-3-oxopropyl]-4-nitrobenzamide

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_N_-[(1_R_,2_S_)-1-(4-Bromophenyl)-2-fluoro-3-(2-methylphenyl)-3-oxopropyl]-4-nitrobenzamide

Crystal data

$C_{23}H_{18}BrFN_2O_4$
M_r = 485.30
Orthorhombic, $P2_12_12$
a = 18.883 (3) Å
b = 21.006 (3) Å
c = 5.3312 (8) Å
V = 2114.6 (5) Å^3
Z = 4
$F(000)$ = 984
D_x = 1.524 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1711 reflections
θ = 4.7–39.6°
μ = 1.99 mm^{-1}
T = 293 K
Prismatic, colorless
0.22 × 0.14 × 0.10 mm

Data collection

Bruker SMART CCD area detector diffractometer
phi and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2007)
T_{min} = 0.528, T_{max} = 0.746
17885 measured reflections
3736 independent reflections
2701 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 25.0°, θ_{min} = 1.5°
h = −22→21
k = −20→24
l = −6→6

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.150
S = 1.13
3736 reflections
285 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0302P)^2 + 2.9914P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}
Absolute structure: Flack x determined using 848 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.008 (19)

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.36145 (6)	0.99683 (5)	0.9915 (3)	0.1162 (5)
F1	0.1370 (2)	0.7403 (3)	1.2524 (9)	0.0816 (15)
N1	0.2301 (4)	0.6919 (4)	0.9107 (14)	0.0550 (17)
N2	0.4240 (5)	0.4409 (4)	1.008 (3)	0.106 (3)
O1	0.0800 (3)	0.6433 (3)	1.0115 (15)	0.0865 (18)
O2	0.2587 (3)	0.6735 (3)	0.5099 (13)	0.0710 (15)
O3	0.4463 (5)	0.4374 (5)	1.221 (3)	0.149 (4)
O4	0.4313 (6)	0.3998 (4)	0.858 (2)	0.167 (5)
C1	−0.0043 (5)	0.7710 (4)	0.6813 (16)	0.071 (2)
H1	0.0117	0.8031	0.7874	0.085*
C2	−0.0520 (4)	0.7856 (5)	0.497 (2)	0.085 (3)
H2	−0.0678	0.8273	0.4773	0.102*
C3	−0.0764 (5)	0.7387 (6)	0.343 (2)	0.087 (3)
H3	−0.1097	0.7480	0.2200	0.104*
C4	−0.0519 (5)	0.6781 (5)	0.370 (2)	0.082 (3)
H4	−0.0684	0.6467	0.2620	0.098*
C5	−0.0032 (4)	0.6617 (4)	0.5536 (15)	0.064 (2)
C6	0.0211 (3)	0.7095 (4)	0.7142 (15)	0.0513 (19)
C7	0.0723 (4)	0.6953 (4)	0.9182 (16)	0.058 (2)
C8	0.1210 (3)	0.7495 (4)	1.0053 (16)	0.0534 (16)
H8	0.0968	0.7904	0.9845	0.064*
C9	0.1898 (4)	0.7495 (3)	0.8539 (13)	0.0465 (17)
H9	0.1771	0.7480	0.6758	0.056*
C10	0.2325 (4)	0.8094 (3)	0.8961 (14)	0.0474 (18)
C11	0.2781 (4)	0.8167 (4)	1.0955 (16)	0.062 (2)
H11	0.2834	0.7840	1.2116	0.075*
C12	0.3163 (5)	0.8729 (5)	1.1241 (18)	0.076 (3)
H12	0.3471	0.8776	1.2589	0.091*
C13	0.3085 (4)	0.9206 (4)	0.955 (2)	0.073 (3)
C14	0.2650 (5)	0.9136 (4)	0.757 (2)	0.081 (3)
H14	0.2607	0.9462	0.6395	0.097*
C15	0.2266 (4)	0.8581 (4)	0.7278 (19)	0.071 (2)
H15	0.1963	0.8538	0.5913	0.085*
C16	0.0228 (6)	0.5939 (4)	0.564 (2)	0.114 (4)
H16A	0.0056	0.5710	0.4210	0.170*
H16B	0.0056	0.5740	0.7148	0.170*
H16C	0.0736	0.5935	0.5646	0.170*
C17	0.2622 (4)	0.6593 (4)	0.7316 (17)	0.0533 (19)
C18	0.3041 (4)	0.6024 (3)	0.8126 (16)	0.055 (2)
C19	0.3049 (5)	0.5494 (4)	0.663 (2)	0.083 (3)
H19	0.2786	0.5489	0.5153	0.100*
C20	0.3442 (6)	0.4969 (5)	0.727 (2)	0.100 (3)
H20	0.3440	0.4609	0.6253	0.120*
C21	0.3828 (4)	0.4981 (4)	0.938 (2)	0.076 (3)
C22	0.3846 (5)	0.5492 (5)	1.088 (2)	0.087 (3)

H22	0.4126	0.5492	1.2312	0.104*
C23	0.3442 (4)	0.6025 (4)	1.026 (2)	0.075 (3)
H23	0.3446	0.6381	1.1299	0.090*
H1A	0.231 (3)	0.683 (3)	1.068 (15)	0.035 (19)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.1014 (7)	0.0852 (7)	0.1621 (12)	−0.0295 (6)	0.0183 (9)	−0.0316 (10)
F1	0.063 (3)	0.135 (5)	0.047 (3)	0.006 (3)	0.002 (2)	−0.003 (3)
N1	0.061 (4)	0.065 (5)	0.039 (4)	0.016 (3)	0.006 (3)	−0.002 (3)
N2	0.099 (6)	0.060 (6)	0.160 (11)	0.023 (5)	0.035 (9)	0.036 (8)
O1	0.092 (4)	0.072 (4)	0.096 (5)	0.005 (3)	−0.010 (5)	0.024 (4)
O2	0.085 (4)	0.074 (4)	0.053 (4)	0.017 (3)	0.002 (4)	−0.001 (4)
O3	0.124 (7)	0.131 (8)	0.192 (12)	0.057 (6)	0.012 (8)	0.065 (9)
O4	0.218 (11)	0.070 (6)	0.212 (12)	0.062 (7)	0.062 (9)	0.029 (7)
C1	0.070 (5)	0.070 (6)	0.073 (6)	0.012 (5)	−0.018 (5)	−0.010 (4)
C2	0.080 (5)	0.088 (6)	0.088 (7)	0.034 (5)	−0.019 (6)	−0.005 (7)
C3	0.061 (5)	0.119 (9)	0.081 (7)	0.017 (6)	−0.019 (5)	−0.009 (7)
C4	0.066 (5)	0.096 (8)	0.083 (7)	−0.022 (5)	−0.016 (5)	−0.012 (6)
C5	0.066 (4)	0.063 (5)	0.064 (6)	−0.016 (4)	0.007 (5)	−0.001 (4)
C6	0.040 (4)	0.056 (5)	0.058 (5)	0.000 (3)	0.002 (3)	0.003 (4)
C7	0.051 (4)	0.057 (5)	0.065 (6)	0.008 (4)	0.002 (4)	0.002 (4)
C8	0.054 (4)	0.063 (4)	0.044 (4)	0.011 (3)	−0.009 (4)	−0.001 (4)
C9	0.053 (4)	0.049 (4)	0.037 (4)	0.006 (3)	−0.005 (3)	0.000 (3)
C10	0.050 (4)	0.051 (4)	0.042 (4)	0.008 (3)	0.004 (3)	−0.004 (3)
C11	0.068 (5)	0.062 (5)	0.057 (6)	−0.003 (4)	−0.006 (4)	0.004 (4)
C12	0.066 (5)	0.099 (7)	0.063 (6)	−0.002 (5)	−0.004 (5)	−0.022 (6)
C13	0.064 (5)	0.072 (6)	0.081 (7)	−0.005 (4)	0.012 (5)	−0.009 (6)
C14	0.096 (6)	0.063 (6)	0.084 (7)	0.001 (5)	−0.004 (6)	0.011 (5)
C15	0.072 (5)	0.068 (6)	0.073 (6)	−0.001 (4)	−0.018 (5)	0.008 (5)
C16	0.162 (11)	0.062 (6)	0.117 (10)	−0.005 (6)	−0.027 (8)	−0.015 (6)
C17	0.048 (4)	0.053 (5)	0.059 (6)	−0.005 (3)	0.002 (4)	0.000 (4)
C18	0.054 (4)	0.040 (4)	0.070 (6)	−0.008 (3)	0.012 (4)	0.001 (4)
C19	0.098 (7)	0.048 (5)	0.103 (8)	0.005 (5)	−0.016 (6)	−0.011 (5)
C20	0.129 (9)	0.043 (5)	0.129 (10)	0.007 (6)	0.005 (8)	−0.012 (7)
C21	0.069 (5)	0.051 (5)	0.108 (9)	0.011 (4)	0.027 (5)	0.015 (6)
C22	0.074 (6)	0.085 (7)	0.103 (9)	0.021 (5)	−0.001 (5)	0.011 (6)
C23	0.074 (5)	0.060 (5)	0.091 (7)	0.014 (4)	−0.006 (6)	−0.012 (5)

Geometric parameters (Å, º)

Br1—C13	1.897 (8)	C9—H9	0.9800
F1—C8	1.365 (9)	C10—C15	1.366 (11)
N1—C17	1.323 (11)	C10—C11	1.377 (11)
N1—C9	1.460 (9)	C11—C12	1.391 (12)
N1—H1A	0.86 (8)	C11—H11	0.9300
N2—O4	1.187 (16)	C12—C13	1.357 (13)

N2—O3	1.209 (17)	C12—H12	0.9300
N2—C21	1.478 (12)	C13—C14	1.348 (14)
O1—C7	1.209 (9)	C14—C15	1.382 (12)
O2—C17	1.220 (10)	C14—H14	0.9300
C1—C2	1.369 (12)	C15—H15	0.9300
C1—C6	1.388 (11)	C16—H16A	0.9600
C1—H1	0.9300	C16—H16B	0.9600
C2—C3	1.362 (13)	C16—H16C	0.9600
C2—H2	0.9300	C17—C18	1.497 (10)
C3—C4	1.362 (13)	C18—C23	1.367 (12)
C3—H3	0.9300	C18—C19	1.372 (11)
C4—C5	1.386 (12)	C19—C20	1.371 (13)
C4—H4	0.9300	C19—H19	0.9300
C5—C6	1.397 (10)	C20—C21	1.343 (14)
C5—C16	1.507 (12)	C20—H20	0.9300
C6—C7	1.486 (11)	C21—C22	1.337 (14)
C7—C8	1.535 (10)	C22—C23	1.395 (12)
C8—C9	1.529 (10)	C22—H22	0.9300
C8—H8	0.9800	C23—H23	0.9300
C9—C10	1.510 (10)		

C17—N1—C9	121.2 (7)	C10—C11—C12	120.3 (8)
C17—N1—H1A	125 (5)	C10—C11—H11	119.8
C9—N1—H1A	114 (5)	C12—C11—H11	119.8
O4—N2—O3	123.2 (12)	C13—C12—C11	119.8 (9)
O4—N2—C21	118.8 (15)	C13—C12—H12	120.1
O3—N2—C21	117.9 (13)	C11—C12—H12	120.1
C2—C1—C6	121.8 (8)	C14—C13—C12	120.4 (9)
C2—C1—H1	119.1	C14—C13—Br1	119.6 (8)
C6—C1—H1	119.1	C12—C13—Br1	119.9 (8)
C3—C2—C1	119.5 (9)	C13—C14—C15	120.0 (9)
C3—C2—H2	120.3	C13—C14—H14	120.0
C1—C2—H2	120.3	C15—C14—H14	120.0
C4—C3—C2	119.8 (9)	C10—C15—C14	121.1 (9)
C4—C3—H3	120.1	C10—C15—H15	119.4
C2—C3—H3	120.1	C14—C15—H15	119.4
C3—C4—C5	122.2 (9)	C5—C16—H16A	109.5
C3—C4—H4	118.9	C5—C16—H16B	109.5
C5—C4—H4	118.9	H16A—C16—H16B	109.5
C4—C5—C6	118.1 (8)	C5—C16—H16C	109.5
C4—C5—C16	118.6 (9)	H16A—C16—H16C	109.5
C6—C5—C16	123.3 (8)	H16B—C16—H16C	109.5
C1—C6—C5	118.6 (7)	O2—C17—N1	123.3 (8)
C1—C6—C7	120.2 (7)	O2—C17—C18	120.2 (8)
C5—C6—C7	121.2 (7)	N1—C17—C18	116.6 (8)
O1—C7—C6	124.1 (7)	C23—C18—C19	118.7 (8)
O1—C7—C8	118.2 (7)	C23—C18—C17	122.1 (7)
C6—C7—C8	117.6 (7)	C19—C18—C17	119.1 (8)

F1—C8—C9	108.7 (5)	C20—C19—C18	120.9 (10)
F1—C8—C7	108.6 (6)	C20—C19—H19	119.5
C9—C8—C7	110.5 (6)	C18—C19—H19	119.5
F1—C8—H8	109.7	C21—C20—C19	119.3 (10)
C9—C8—H8	109.7	C21—C20—H20	120.4
C7—C8—H8	109.7	C19—C20—H20	120.4
N1—C9—C10	112.4 (6)	C22—C21—C20	121.8 (9)
N1—C9—C8	109.4 (6)	C22—C21—N2	119.3 (12)
C10—C9—C8	112.0 (6)	C20—C21—N2	118.9 (11)
N1—C9—H9	107.6	C21—C22—C23	119.5 (10)
C10—C9—H9	107.6	C21—C22—H22	120.3
C8—C9—H9	107.6	C23—C22—H22	120.3
C15—C10—C11	118.3 (7)	C18—C23—C22	119.9 (9)
C15—C10—C9	118.9 (7)	C18—C23—H23	120.1
C11—C10—C9	122.8 (7)	C22—C23—H23	120.1

C6—C1—C2—C3	0.9 (15)	C9—C10—C11—C12	179.7 (7)
C1—C2—C3—C4	−1.4 (16)	C10—C11—C12—C13	0.1 (13)
C2—C3—C4—C5	1.1 (16)	C11—C12—C13—C14	−1.2 (14)
C3—C4—C5—C6	−0.2 (14)	C11—C12—C13—Br1	−179.3 (6)
C3—C4—C5—C16	−178.1 (10)	C12—C13—C14—C15	1.5 (15)
C2—C1—C6—C5	0.0 (13)	Br1—C13—C14—C15	179.5 (7)
C2—C1—C6—C7	−179.3 (8)	C11—C10—C15—C14	−0.5 (13)
C4—C5—C6—C1	−0.4 (11)	C9—C10—C15—C14	−179.5 (8)
C16—C5—C6—C1	177.4 (9)	C13—C14—C15—C10	−0.6 (15)
C4—C5—C6—C7	178.9 (8)	C9—N1—C17—O2	−2.3 (12)
C16—C5—C6—C7	−3.3 (12)	C9—N1—C17—C18	177.8 (6)
C1—C6—C7—O1	155.6 (9)	O2—C17—C18—C23	140.8 (8)
C5—C6—C7—O1	−23.7 (12)	N1—C17—C18—C23	−39.3 (10)
C1—C6—C7—C8	−27.8 (10)	O2—C17—C18—C19	−36.2 (11)
C5—C6—C7—C8	152.9 (7)	N1—C17—C18—C19	143.7 (9)
O1—C7—C8—F1	−32.7 (10)	C23—C18—C19—C20	1.2 (14)
C6—C7—C8—F1	150.5 (6)	C17—C18—C19—C20	178.3 (9)
O1—C7—C8—C9	86.5 (9)	C18—C19—C20—C21	−0.8 (16)
C6—C7—C8—C9	−90.3 (7)	C19—C20—C21—C22	−0.5 (16)
C17—N1—C9—C10	−97.0 (8)	C19—C20—C21—N2	179.0 (9)
C17—N1—C9—C8	137.8 (7)	O4—N2—C21—C22	−168.2 (10)
F1—C8—C9—N1	52.9 (8)	O3—N2—C21—C22	14.7 (15)
C7—C8—C9—N1	−66.3 (8)	O4—N2—C21—C20	12.3 (14)
F1—C8—C9—C10	−72.5 (7)	O3—N2—C21—C20	−164.8 (11)
C7—C8—C9—C10	168.4 (6)	C20—C21—C22—C23	1.3 (15)
N1—C9—C10—C15	139.4 (7)	N2—C21—C22—C23	−178.1 (8)
C8—C9—C10—C15	−96.9 (8)	C19—C18—C23—C22	−0.3 (13)
N1—C9—C10—C11	−39.5 (9)	C17—C18—C23—C22	−177.3 (8)
C8—C9—C10—C11	84.2 (8)	C21—C22—C23—C18	−0.9 (14)
C15—C10—C11—C12	0.7 (12)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···F1	0.86 (8)	2.36 (6)	2.728 (9)	106 (5)
N1—H1*A*···O2^{i}	0.86 (8)	2.42 (8)	3.263 (10)	166 (4)
C9—H9···F1^{ii}	0.98	2.39	3.364 (8)	175
C8—H8···O4^{iii}	0.98	2.50	3.387 (12)	150
C9—H9···O2	0.98	2.37	2.758 (9)	103

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