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Synthesis and crystal structure of (*E*)-*N*-[(2-bromophenyl)methylidene]-3,5-bis(trifluoromethyl) aniline

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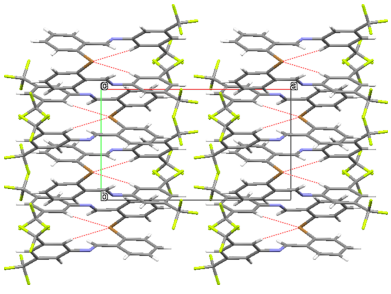
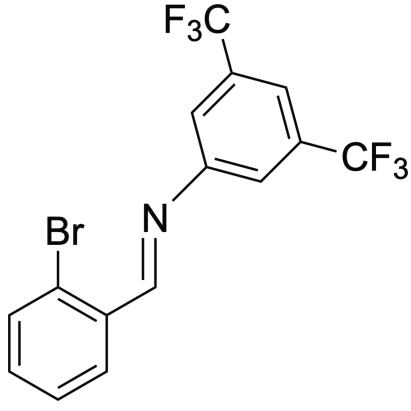
The title compound $C_{15}H_8BrF_6N$, was prepared by a condensation reaction of 2-bromobenzaldehyde and 3,5-bis(trifluoromethyl)aniline in the presence of anhydrous magnesium sulfate. The compound readily crystallizes from a concentrated hexanes solution in high yield. The imine bond is nearly planar with the 2-bromophenyl group, while the *N*-(3,5-bis(trifluoromethyl)phenyl moiety is significantly twisted from the imine group [49.61 (5)°]. The crystal packing involves short intermolecular C—H···Br contacts linking zigzag ribbons flanked by fluorous layers.

1. Chemical context

Arylimine-type ligands have increasingly been used as ancillary ligands for a variety of metal complexes. (Dostál *et al.*, 2011; Hejda *et al.*, 2012; Hejda *et al.*, 2013, 2017; Joseph *et al.*, 2018; Kingsley *et al.*, 2016; Kořenková *et al.*, 2016; Kremláček *et al.*, 2018; Mungwe *et al.*, 2011; Novák *et al.*, 2014, 2016; Šimon *et al.*, 2013; Urbanová *et al.*, 2013, 2014; Vrána *et al.*, 2013; Zhao *et al.*, 2010, 2011) Synthesis of these ligands is typically performed with alkyl-substituted anilines or alkyl amines reacting with 2-brombenzaldehyde. There is interest in modifying the electronic structure of the ligands but this has been limited to substitutions on the aromatic ring of the benzaldehyde starting material. (Chen *et al.*, 2004; Li *et al.*, 2019). Our group is interested in developing arylimine ligands with electron-withdrawing groups on the aromatic ring of the *N*-imine portion of the ligand. Herein we report the synthesis and crystal structure of (*E*)-*N*-[(2-bromophenyl)methylidene]-3,5-bis(trifluoromethyl)aniline (**I**).





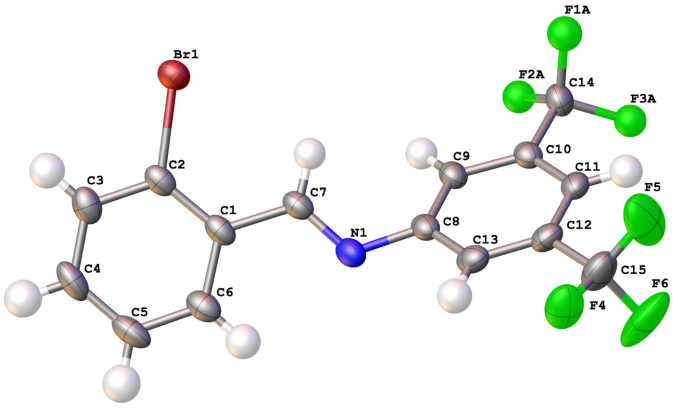


Figure 1
The molecular structure of **I**. Only one of the three CF_3 disorder model conformations shown. Thermal displacement ellipsoids are drawn at the 50% probability level.

2. Structural commentary

A displacement ellipsoid plot of compound **I** is shown in Fig. 1. The imine bond length C7—N1 [1.280 (4) Å] and C7—N1—C8 bond angle [119.1 (2)°] are consistent with atom N1 being sp^2 hybridized. The imine bond is oriented nearly coplanar with the C1–C6 phenyl ring [angle between least squares planes formed by C1–C6 and N1,C7,C1 = 5.9 (3)°]. Torsion angles (Table 1) near the imine bond demonstrate this as well as the twist of the C8–C13 phenyl ring relative to the imine bond plane formed by C8/N1/C7 is 42.0 (3)°). The angle between the least-squares planes formed by C1–C8/N1/Br1 and C8–C15/N1 of 49.61 (5)° is consistent with steric limitations influenced by atom positions of H7 and H9. Short intramolecular interactions involving C—H bonds with acceptors are also present. A short C7—H7···Br1 contact (2.82 Å, length − vdW radii sums = −0.244 Å) and another contact involving C6—H6···N1 (2.52 Å, length − vdW sums = −0.342 Å) help define the observed conformation of **I** (Table 2).

Table 1
Selected torsion angles (°).

C2—C1—C7—N1	174.5 (2)	C7—N1—C8—C13	139.5 (3)
C6—C1—C7—N1	−5.9 (4)	C8—N1—C7—C1	176.7 (2)
C7—N1—C8—C9	−43.7 (4)		

3. Supramolecular features

While no conventional hydrogen-bonding interactions are present, several short C—H···F contacts with fluorine atoms of the disordered CF_3 group and hydrogen atoms H3 and H4 are present (Table 2, Fig. 2). A contact involving C13—H13···Br1 is also present, forming zigzag infinite ribbons of molecules along (001) as shown in Fig. 3. The packing diagram of **I** (Fig. 4) demonstrates how the CF_3 groups associate in fluorous layers in the *bc* plane at x = 0.5

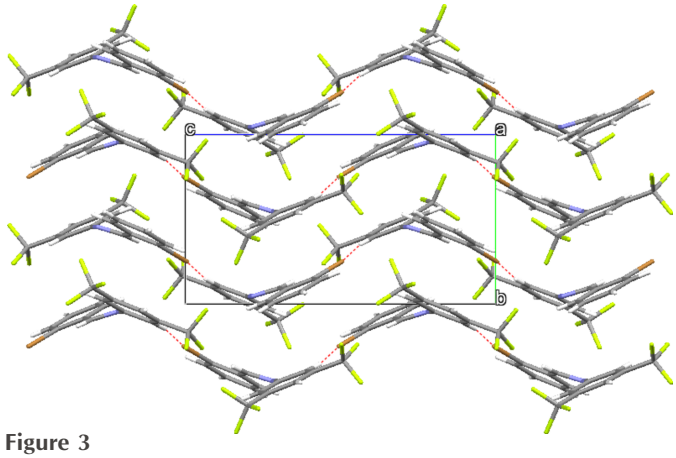


Figure 3
Packing diagram of **I** in a view along the *a*-axis direction. C—H···Br interactions are shown as dashed lines.

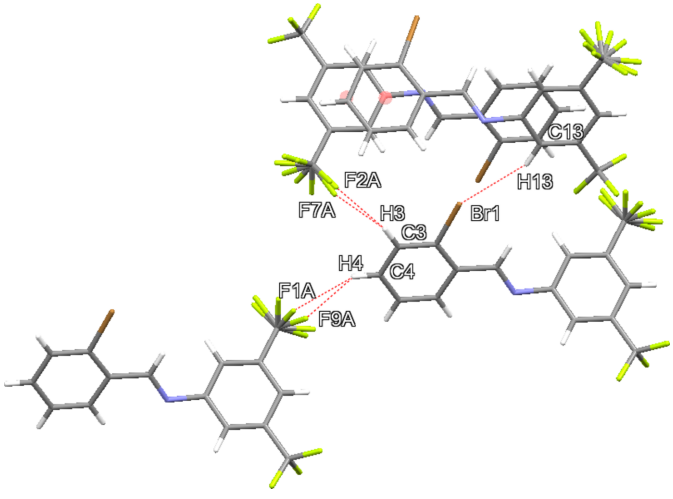


Figure 2
Intermolecular interactions of **I** including centroids of the weak π–π dimer.

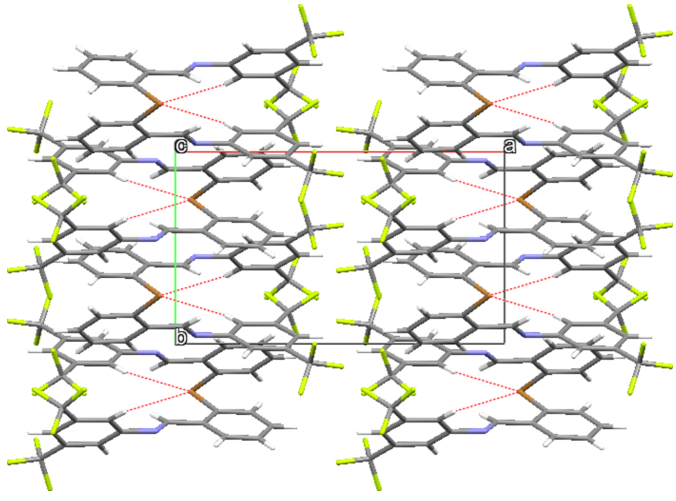


Figure 4
Packing diagram of **I** in a view along the *c*-axis direction. C—H···Br interactions are shown as dashed lines.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···F2A^{i}	0.95	2.46	3.365 (7)	160
C3—H3···F7A^{i}	0.95	2.25	3.063 (7)	143
C4—H4···F1A^{ii}	0.95	2.54	3.411 (6)	153
C4—H4···F9A^{ii}	0.95	2.36	3.152 (9)	140
C6—H6···N1	0.95	2.52	2.828 (4)	99
C7—H7···Br1	0.95	2.82	3.233 (3)	108
C13—H13···Br1^{iii}	0.95	2.97	3.851 (3)	155

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

with the ribbons of C—H···Br interactions between the CF_3-rich layers. Weak π–π dimer intermolecular interactions between a neighboring brominated phenyl ring (less electron poor) and the trifluoromethylated phenyl ring (more electron poor) are evident, with a 3.730 (2) Å centroid-to-centroid distance.

4. Database survey

A recent search in the CSD (version 6.00, last update April 2025; Groom *et al.*, 2016) using ConQuest (Bruno *et al.*, 2002) revealed the most closely related structures to **I** include a single *meta*-fluoro substitution (in place of a bis-trifluoromethyl-substituted phenyl ring). The structure of 1-(2-bromophenyl)-*N*-(3-fluorophenyl)methanimine (FOBLUF; Kaur & Choudhury, 2014) demonstrates similar intramolecular features to **I**, including the imine C—H···Br and phenyl *ortho* C—H···N distances (2.76 and 2.53 Å, respectively) as well as the twist angle between phenyl least-squares planes [40.97 (8)°]. Another related structure reported with a single electron-withdrawing *meta* substituent on the *N*-imine ring is *N*-(2-iodobenzylidene)-3-nitroaniline (MOPPOW; Wardell *et al.*, 2002). Similar to **I**, this mono-nitro-substituted structure also demonstrates analogous phenyl *ortho* C—H···N distances (2.58 Å) but the twist angle between phenyl least-squares planes (64.2°) is significantly different and may be related to the presence of the intermolecular halogen bonding that is present (I···N distance = 3.487 Å, C8—I1···N1 = 160.1°). The structure of 2-({[3,5-bis(trifluoromethyl)phenyl]imino}methyl)-5-(dimethylamino)phenol (BIDCUQ; Zhao *et al.*, 2023) possesses the same 3,5-bis(trifluoromethyl)phenyl moiety as **I**, but the imine-linked 2-hydroxy phenyl group engages an intramolecular interaction (O1—H1···N2 = 1.84 Å), inducing a coplanar orientation of the phenyl rings. Also, the CF_3 groups of BIDCUQ associate in fluorous layers (similar to **I**) between infinite single-distance π–π stacked aromatic regions (3.47 Å).

5. Synthesis and crystallization

2-Bromobenzaldehyde (4.50 g, 24.3 mmol) was stirred in hexanes (250 mL) in the presence of anhydrous $MgSO_4$ (1.0 g). 3,5-Bis(trifluoromethyl)aniline (5.575 g, 24.3 mmol) was slowly added and the solution was allowed to stir for 2 h. $MgSO_4$ was then removed via vacuum filtration and the filtrate cooled to 243 K for 48 h. The yellow precipitate was collected via vacuum filtration and purified through recrystallization from hexanes. The resulting material was light-yellow and crystalline. Yield: 7.62 g, 79%. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.86 (*s*, 1H, C*H*═N), 8.22 (*dd*, $^3J_{HH}$ = 7.7 Hz, $^4J_{HH}$ = 1.9 Hz 1H, aryl H6), 7.76 (*br s*, 1H, aryl H11), 7.66 (*dd*, $^3J_{HH}$ = 7.7 Hz, $^4J_{HH}$ = 1.9 Hz 1H, aryl H3), 7.63 (*br s*, 2H, aryl H9, H13), 7.44 (*m*, 1H, aryl H5), 7.38 (*m*, 1H, aryl H4). ^{13}C NMR {^{1}H} ($CDCl_3$, 100 MHz): δ 162.30 (*s*, C7), 153.15 (*s*, aryl C8), 133.81 (*s*, aryl C1), 133.62 (*s*, aryl C4), 133.58 (*s*, aryl C3), 132.79 (*q*, $^2J_{CF}$ = 33.6 Hz, aryl C10, C12), 129.41 (*s*, aryl C6), 128.05 (*s*, aryl C5), 126.71 (*s*, aryl C2), 123.32 (*q*, $^1J_{CF}$ = 272.8 Hz, C14, C15), 121.40 (*q*, $^3J_{CF}$ = 2.7 Hz, aryl C9, C13), 119.71 (sept, $^3J_{CF}$ = 3.8 Hz, aryl C11). M.p.: 361–363 K. X-ray quality crystals were grown from a concentrated solution in warm hexanes followed by slow cooling to room temperature and storage at 243 K for 96 h.

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_8BrF_6N$
M_r	396.13
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	13.261 (2), 7.7224 (12), 14.176 (2)
β (°)	93.394 (2)
V (Å^3)	1449.2 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	2.90
Crystal size (mm)	0.25 × 0.20 × 0.15
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.575, 0.747
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	23866, 5193, 3166
R_{int}	0.053
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.766
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.046, 0.137, 1.06
No. of reflections	5193
No. of parameters	217
No. of restraints	189
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.89, −0.68

Computer programs: *APEX2* and *SAINT* (Bruker 2017), *SHELXS97* (Sheldrick, 2008), *SHELXL2019/2* (Sheldrick, 2015), *OLEX2* (Dolomanov *et al.*, 2009), *Mercury* (Macrae *et al.*, 2020) and *publCIF* (Westrip, 2010).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. Hydrogen atoms were refined with riding coordinates with fixed U_{iso}(H) at 1.2 times of the riding C atom. Several restraints and constraints were used to model disorder in one of the CF_3 groups. Distance restraints were employed for C14—F1*A*, C14—F2*A*, C14—F3*A*, C14—F4*A*, C14—F5*A*, C14—F6*A*, C14—F7*A*, C14—F8*A*, and C14—F9*A* with sigma of 0.02; F1*A*—F2*A*, F2*A*—F3*A*, F3*A*—F1*A*, F4*A*—F5*A*, F5*A*—F6*A*, F6*A*—F4*A*, F7*A*—F8*A*, F8*A*—F9*A*,

and F9*A*—F7*A* with sigma of 0.04; and C10—F1*A*, C10—F2*A*, C10—F3*A*, C10—F4*A*, C10—F5*A*, C10—F6*A*, C10—F7*A*, C10—F8*A*, and C10—F9*A* with sigma of 0.1. U_{aniso} restraints were applied to C10, C14, F1*A*, F2*A*, F3*A*, F4*A*, F5*A*, F6*A*, F7*A*, F8*A*, and F9*A* within 2 Å with sigma of 0.04 and sigma for terminal atoms of 0.08 within 2 Å. Rigid body (RIGU) restraints were applied to C10, C14, F1*A*, F2*A*, F3*A*, F4*A*, F5*A*, F6*A*, F7*A*, F8*A*, F9*A* with sigma for 1–2 distances of 0.004 and sigma for 1–3 distances of 0.004. The three orientations of the CF_3 group were fixed at sof values of 0.37 (F1*A*, F2*A*, F3*A*), 0.38 (F4*A*, F5*A*, F6*A*), and 0.25 (F7*A*, F8*A*, F9*A*).

Acknowledgements

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Computing details

(*E*)-*N*-[(2-Bromophenyl)methylidene]-3,5-bis(trifluoromethyl)aniline

Crystal data

$C_{15}H_8BrF_6N$
$M_r = 396.13$
Monoclinic, $P2_1/c$
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$b = 7.7224$ (12) Å
$c = 14.176$ (2) Å
$\beta = 93.394$ (2)°
$V = 1449.2$ (4) Å^3
$Z = 4$
$F(000) = 776$
$D_x = 1.816$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6800 reflections
$\theta = 2.9$–31.3°
$\mu = 2.90$ mm^{-1}
$T = 100$ K
Irregular brick, yellow
0.25 × 0.20 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: sealed tube
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
$T_{min} = 0.575$, $T_{max} = 0.747$
23866 measured reflections
5193 independent reflections
3166 reflections with $I > 2\sigma(I)$
$R_{int} = 0.053$
$\theta_{max} = 33.0°$, $\theta_{min} = 2.9°$
$h = -20\rightarrow19$
$k = -11\rightarrow11$
$l = -21\rightarrow21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.137$
$S = 1.06$
5193 reflections
217 parameters
189 restraints
Primary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0521P)^2 + 1.1524P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.89$ e Å^{-3}
$\Delta\rho_{min} = -0.68$ e Å^{-3}

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}	Occ. (<1)
Br1	−0.04663 (2)	0.75027 (4)	−0.00485 (2)	0.03627 (10)	
N1	0.05952 (17)	0.5457 (3)	0.28171 (18)	0.0335 (5)	
C1	−0.08432 (19)	0.5863 (3)	0.1738 (2)	0.0288 (5)	
C2	−0.12674 (19)	0.6484 (3)	0.08793 (19)	0.0293 (5)	
C3	−0.2302 (2)	0.6421 (4)	0.0656 (2)	0.0363 (6)	
H3	−0.257428	0.686307	0.006931	0.044*	
C4	−0.2931 (2)	0.5709 (4)	0.1295 (2)	0.0409 (7)	
H4	−0.363907	0.565656	0.114812	0.049*	
C5	−0.2530 (2)	0.5069 (4)	0.2152 (3)	0.0415 (7)	
H5	−0.296289	0.457257	0.258939	0.050*	
C6	−0.1504 (2)	0.5155 (3)	0.2369 (2)	0.0349 (6)	
H6	−0.123955	0.472455	0.296075	0.042*	
C7	0.02492 (19)	0.5917 (3)	0.1993 (2)	0.0289 (5)	
H7	0.070172	0.629651	0.154103	0.035*	
C8	0.16523 (19)	0.5438 (3)	0.3021 (2)	0.0297 (5)	
C9	0.23302 (19)	0.4776 (3)	0.2399 (2)	0.0288 (5)	
H9	0.209397	0.434980	0.179772	0.035*	
C10	0.33567 (19)	0.4746 (3)	0.26672 (19)	0.0290 (5)	
C11	0.3715 (2)	0.5378 (3)	0.35389 (19)	0.0317 (5)	
H11	0.441795	0.536850	0.371320	0.038*	
C12	0.3035 (2)	0.6022 (4)	0.41483 (19)	0.0346 (6)	
C13	0.2009 (2)	0.6037 (4)	0.3903 (2)	0.0350 (6)	
H13	0.154798	0.645660	0.433828	0.042*	
C14	0.4097 (2)	0.4018 (4)	0.2017 (2)	0.0355 (6)	
F1A	0.4543 (5)	0.5294 (7)	0.1579 (5)	0.0421 (12)*	0.37
F2A	0.3653 (4)	0.2903 (8)	0.1396 (4)	0.0366 (12)*	0.37
F3A	0.4837 (4)	0.3151 (8)	0.2533 (3)	0.0359 (11)*	0.37
F4A	0.4225 (4)	0.4969 (7)	0.1218 (4)	0.0469 (12)*	0.38
F5A	0.3808 (4)	0.2437 (6)	0.1641 (4)	0.0375 (11)*	0.38
F6A	0.5052 (4)	0.3815 (7)	0.2361 (4)	0.0438 (12)*	0.38
F7A	0.3694 (5)	0.3701 (10)	0.1145 (4)	0.0354 (14)*	0.25
F8A	0.4543 (7)	0.2606 (11)	0.2394 (6)	0.049 (2)*	0.25
F9A	0.4841 (7)	0.5119 (11)	0.1888 (7)	0.055 (2)*	0.25
C15	0.3438 (3)	0.6664 (6)	0.5095 (2)	0.0547 (9)	
F4	0.27725 (19)	0.7607 (3)	0.55397 (15)	0.0614 (6)	
F5	0.4281 (2)	0.7610 (4)	0.50321 (19)	0.0861 (10)	
F6	0.3718 (2)	0.5370 (4)	0.56638 (16)	0.0989 (10)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.03181 (15)	0.04145 (16)	0.03619 (15)	0.00118 (12)	0.00736 (10)	0.00104 (12)
N1	0.0269 (11)	0.0333 (12)	0.0412 (12)	0.0038 (9)	0.0078 (9)	0.0063 (10)
C1	0.0238 (11)	0.0230 (11)	0.0405 (14)	−0.0009 (9)	0.0086 (10)	−0.0062 (10)
C2	0.0259 (12)	0.0251 (11)	0.0377 (14)	0.0000 (9)	0.0088 (10)	−0.0087 (10)
C3	0.0284 (13)	0.0351 (13)	0.0452 (16)	0.0030 (11)	0.0011 (11)	−0.0102 (12)
C4	0.0215 (12)	0.0402 (15)	0.062 (2)	−0.0021 (11)	0.0078 (12)	−0.0148 (14)
C5	0.0310 (15)	0.0332 (14)	0.063 (2)	−0.0032 (11)	0.0217 (14)	−0.0041 (14)
C6	0.0315 (14)	0.0265 (12)	0.0479 (16)	−0.0001 (10)	0.0120 (12)	−0.0021 (11)
C7	0.0257 (11)	0.0238 (11)	0.0380 (14)	−0.0006 (9)	0.0086 (10)	−0.0016 (10)
C8	0.0265 (12)	0.0274 (12)	0.0357 (13)	0.0010 (9)	0.0049 (10)	0.0085 (10)
C9	0.0253 (12)	0.0276 (12)	0.0339 (13)	−0.0014 (9)	0.0041 (10)	0.0035 (10)
C10	0.0269 (12)	0.0269 (11)	0.0336 (13)	−0.0008 (9)	0.0042 (10)	0.0052 (10)
C11	0.0309 (13)	0.0309 (13)	0.0329 (13)	−0.0003 (10)	−0.0005 (10)	0.0104 (10)
C12	0.0421 (15)	0.0353 (14)	0.0262 (12)	0.0044 (11)	0.0008 (11)	0.0072 (10)
C13	0.0380 (15)	0.0351 (14)	0.0324 (13)	0.0082 (11)	0.0074 (11)	0.0085 (11)
C14	0.0257 (12)	0.0401 (15)	0.0406 (15)	−0.0003 (10)	0.0004 (11)	0.0021 (12)
C15	0.059 (2)	0.072 (2)	0.0316 (16)	0.0147 (19)	−0.0048 (15)	0.0031 (16)
F4	0.0617 (14)	0.0846 (17)	0.0374 (10)	0.0156 (11)	−0.0001 (9)	−0.0144 (10)
F5	0.0564 (14)	0.144 (3)	0.0563 (15)	−0.0185 (15)	−0.0079 (11)	−0.0325 (15)
F6	0.139 (3)	0.119 (2)	0.0364 (12)	0.058 (2)	−0.0165 (14)	0.0149 (13)

Geometric parameters (Å, º)

Br1—C2	1.908 (3)	C10—C11	1.386 (4)
N1—C7	1.280 (4)	C10—C14	1.496 (4)
N1—C8	1.414 (3)	C11—H11	0.9500
C1—C2	1.396 (4)	C11—C12	1.378 (4)
C1—C6	1.400 (4)	C12—C13	1.384 (4)
C1—C7	1.473 (4)	C12—C15	1.499 (4)
C2—C3	1.391 (4)	C13—H13	0.9500
C3—H3	0.9500	C14—F1A	1.323 (6)
C3—C4	1.382 (4)	C14—F2A	1.342 (5)
C4—H4	0.9500	C14—F3A	1.364 (5)
C4—C5	1.388 (5)	C14—F4A	1.369 (5)
C5—H5	0.9500	C14—F5A	1.377 (5)
C5—C6	1.379 (4)	C14—F6A	1.338 (5)
C6—H6	0.9500	C14—F7A	1.339 (6)
C7—H7	0.9500	C14—F8A	1.336 (7)
C8—C9	1.392 (4)	C14—F9A	1.323 (8)
C8—C13	1.390 (4)	C15—F4	1.331 (4)
C9—H9	0.9500	C15—F5	1.343 (5)
C9—C10	1.392 (3)	C15—F6	1.324 (4)
C7—N1—C8	119.1 (2)	C12—C11—C10	118.9 (3)
C2—C1—C6	117.2 (2)	C12—C11—H11	120.5

C2—C1—C7	122.9 (2)	C11—C12—C13	121.1 (3)
C6—C1—C7	119.9 (3)	C11—C12—C15	117.9 (3)
C1—C2—Br1	122.07 (19)	C13—C12—C15	121.0 (3)
C3—C2—Br1	116.1 (2)	C8—C13—H13	120.0
C3—C2—C1	121.8 (3)	C12—C13—C8	120.0 (3)
C2—C3—H3	120.3	C12—C13—H13	120.0
C4—C3—C2	119.4 (3)	F1A—C14—C10	109.7 (3)
C4—C3—H3	120.3	F1A—C14—F2A	111.2 (4)
C3—C4—H4	120.0	F1A—C14—F3A	106.9 (4)
C3—C4—C5	120.1 (3)	F2A—C14—C10	111.5 (3)
C5—C4—H4	120.0	F2A—C14—F3A	108.1 (4)
C4—C5—H5	120.0	F3A—C14—C10	109.3 (3)
C6—C5—C4	120.0 (3)	F4A—C14—C10	115.2 (3)
C6—C5—H5	120.0	F4A—C14—F5A	101.6 (4)
C1—C6—H6	119.2	F5A—C14—C10	113.2 (3)
C5—C6—C1	121.6 (3)	F6A—C14—C10	117.4 (3)
C5—C6—H6	119.2	F6A—C14—F4A	101.7 (4)
N1—C7—C1	120.7 (2)	F6A—C14—F5A	105.9 (4)
N1—C7—H7	119.7	F7A—C14—C10	113.4 (3)
C1—C7—H7	119.7	F8A—C14—C10	110.5 (4)
C9—C8—N1	123.0 (3)	F8A—C14—F7A	111.3 (5)
C13—C8—N1	117.4 (2)	F9A—C14—C10	111.4 (4)
C13—C8—C9	119.6 (2)	F9A—C14—F7A	104.5 (6)
C8—C9—H9	120.3	F9A—C14—F8A	105.3 (6)
C10—C9—C8	119.4 (3)	F4—C15—C12	113.2 (3)
C10—C9—H9	120.3	F4—C15—F5	108.2 (3)
C9—C10—C14	120.4 (2)	F5—C15—C12	112.0 (3)
C11—C10—C9	121.0 (2)	F6—C15—C12	111.6 (3)
C11—C10—C14	118.6 (2)	F6—C15—F4	107.1 (3)
C10—C11—H11	120.6	F6—C15—F5	104.3 (3)

Br1—C2—C3—C4	−179.7 (2)	C9—C10—C14—F5A	−47.6 (4)
N1—C8—C9—C10	−177.6 (2)	C9—C10—C14—F6A	−171.5 (4)
N1—C8—C13—C12	178.9 (2)	C9—C10—C14—F7A	10.2 (5)
C1—C2—C3—C4	−0.6 (4)	C9—C10—C14—F8A	−115.5 (5)
C2—C1—C6—C5	0.2 (4)	C9—C10—C14—F9A	127.7 (5)
C2—C1—C7—N1	174.5 (2)	C10—C11—C12—C13	0.3 (4)
C2—C3—C4—C5	0.2 (4)	C10—C11—C12—C15	178.7 (3)
C3—C4—C5—C6	0.4 (4)	C11—C10—C14—F1A	−79.9 (4)
C4—C5—C6—C1	−0.7 (4)	C11—C10—C14—F2A	156.5 (4)
C6—C1—C2—Br1	179.45 (19)	C11—C10—C14—F3A	37.0 (4)
C6—C1—C2—C3	0.4 (4)	C11—C10—C14—F4A	−111.5 (4)
C6—C1—C7—N1	−5.9 (4)	C11—C10—C14—F5A	132.2 (3)
C7—N1—C8—C9	−43.7 (4)	C11—C10—C14—F6A	8.3 (5)
C7—N1—C8—C13	139.5 (3)	C11—C10—C14—F7A	−170.0 (4)
C7—C1—C2—Br1	−0.9 (3)	C11—C10—C14—F8A	64.3 (5)
C7—C1—C2—C3	−179.9 (2)	C11—C10—C14—F9A	−52.5 (6)
C7—C1—C6—C5	−179.5 (3)	C11—C12—C13—C8	−1.7 (4)

C8—N1—C7—C1	176.7 (2)	C11—C12—C15—F4	165.6 (3)
C8—C9—C10—C11	−0.6 (4)	C11—C12—C15—F5	43.0 (4)
C8—C9—C10—C14	179.1 (2)	C11—C12—C15—F6	−73.5 (4)
C9—C8—C13—C12	2.0 (4)	C13—C8—C9—C10	−0.8 (4)
C9—C10—C11—C12	0.9 (4)	C13—C12—C15—F4	−16.0 (5)
C9—C10—C14—F1A	100.3 (4)	C13—C12—C15—F5	−138.6 (3)
C9—C10—C14—F2A	−23.2 (5)	C13—C12—C15—F6	104.9 (4)
C9—C10—C14—F3A	−142.7 (4)	C14—C10—C11—C12	−178.9 (2)
C9—C10—C14—F4A	68.7 (4)	C15—C12—C13—C8	179.9 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···F2*A*^{i}	0.95	2.46	3.365 (7)	160
C3—H3···F7*A*^{i}	0.95	2.25	3.063 (7)	143
C4—H4···F1*A*^{ii}	0.95	2.54	3.411 (6)	153
C4—H4···F9*A*^{ii}	0.95	2.36	3.152 (9)	140
C6—H6···N1	0.95	2.52	2.828 (4)	99
C7—H7···Br1	0.95	2.82	3.233 (3)	108
C13—H13···Br1^{iii}	0.95	2.97	3.851 (3)	155

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