The 1H-pyrazolo[3,4-b]quinoline (PQ) core of the title molecule, C23H14F3N3, is aromatic and essentially planar (r.m.s. deviation = 0.015 Å) and the two phenyl substituents at positions 1 and 3 are twisted relative to this fragment by 29.74 (7) and 25.63 (7)°, respectively. In the crystal, molecules are arranged along the b axis into stacks via π–π interactions, with an interplanar distance of the PQ core of 3.489 (4) Å.

**Related literature**

For selected photophysical properties of trifluoromethyl derivatives of 1H-pyrazolo-[3,4-b]quinoline, see: Koścień, Gondek, Jarosz et al. (2009); Koścień, Gondek, Pokladko et al. (2009). For the use of trifluoromethyl derivatives of 1H-pyrazolo-[3,4-b]quinoline in organic light-emitting diode (OLED) preparation, see: Tao et al. (2001). For the synthesis of 1H-pyrazolo-[3,4-b]quinoline derivatives, see: Brack (1965).
1,3-Diphenyl-8-trifluoromethyl-1\textit{H}-pyrazolo[3,4-\textit{b}]quinoline

Pawel Szlachcic and Katarzyna Stadnicka

S1. Comment

The derivatives of 1\textit{H}-pyrazolo[3,4-\textit{b}]quinoline (PQ) containing trifluoromethyl substituents at C7 were found to have interesting photophysical properties (Koścień, Gondek, Jarosz et al., 2009; Koścień, Gondek, Pokladko et al., 2009). A relatively high quantum efficiency allowed to propose the CF\textsubscript{3} derivatives as blue-light luminophore and to use the derivatives as the chromophore for organic light-emitting diodes (OLED). To synthesize PQ derivatives with H atom in C-4 position, a known method of preparation was used (Brack, 1965). Previously it was found, that in the case of 7-trifluoromethyl-1-methyl-3-phenyl-1\textit{H}-pyrazolo[3,4-\textit{b}]quinoline, the incorporation of CF\textsubscript{3} substituent into PQ molecule raises the values of HOMO/LUMO and ionization potential of the luminophore in comparison to PQ itself (Tao et al., 2001), so 8-trifluoromethyl-1,3-diphenyl-1\textit{H}-pyrazolo[3,4-\textit{b}]quinoline was synthesized as the compound promising useful properties for the construction of OLED cells with Mg/Ag alloy kathode or even Al kathode. The results of using the trifluoromethyl derivatives of 1,3-diphenyl-1\textit{H}-pyrazolo[3,4-\textit{b}]quinoline for OLED preparation will be published elsewhere.

The shape of the title molecule is shown in Fig. 1. The core of the molecule, 1\textit{H}-pyrazolo[3,4-\textit{b}]quinoline, is planar and aromatic. Although the planes of both phenyl substituents should be coplanar with the core moiety (due to the conjugation between aromatic core and aromatic phenyl rings), they are slightly twisted with the torsion angles N2—N1—C11—C16 = 27.6 (4), N2—C3—C31—C32 = -23.9 (4)°. In the case of the phenyl substituent at C3 the effect is caused by the steric hindrance between the hydrogen atoms H4 and H36 (H4···H36 = 2.26 Å). The overall shape of the molecule is also influenced by weak intramolecular interaction C12—H12···N9 (Table 1). The trifluoromethyl group forms two hydrogen-bond-like intermolecular interactions of C—H···F type: intramolecular one C7—H7···F83 and intermolecular one C36—H36···F82 (\(-x, y + 1/2, -z + 1\)) with the geometrical parameters given in Table 1.

The packing of the molecules (Fig. 2 and Fig. 3) is determined mainly by intermolecular \(\pi\)--\(\pi\) stacking with the geometry given below (Cg···Cg···Cg/Å, <CgCgCg/°, respectively):

- Cg3(C4a—C5—C6—C7—C8—C8a at \(-x, y - 1/2, -z + 1\))···Cg1(N1—N2—C3—C3a—C9a)···Cg3(C4a—C5—C6—C7—C8—C8a at \(-x, y + 1/2, -z + 1\)): 3.751 (4), 3.906 (5), 131.4 (3);
- Cg2(C3a—C4—C4a—C8a—N9—C9a at \(-x, y - 1/2, -z + 1\))···Cg2(C3a—C4—C4a—C8a—N9—C9a)···Cg2(C3a—C4—C4a—C8a—N9—C9a): 3.799 (4), 3.799 (4), 133.5 (3);
- Cg3(C4a—C5—C6—C7—C8—C8a at \(-x, y - 1/2, -z + 1\))···Cg2(C3a—C4—C4a—C8a—N9—C9a)···Cg3(C4a—C5—C6—C7—C8—C8a at \(-x, y + 1/2, -z + 1\)): 3.732 (4), 3.787 (4), 136.3 (3).

The structure is additionally stabilized by two C—H···\(\pi\) interactions: C13—H13···Cg4 (\(-x, y + 1/2, -z + 2\)) and C33—H33···Cg4 (\(-x - 1, y - 1/2, -z + 1/2\)) given in Table 1.
S2. Experimental

The title compound was synthesized using procedure already described in literature (Brack, 1965) from 2-(trifluoromethyl)aniline and 5-chloro-1,3-diphenyl-1H-pyrazol-4-carbaldehyde (5 mmol of each substrate, sulfolane as a solvent). The product was purified by column chromatography (SilicaGel 60, toluene/petroleum ether 1:1 as the eluent) followed by preparative TLC (SilicaGel 60, 2 mm, toluene/petroleum ether 1:1 as the eluent) to give 50 mg (2.6% yield - the low yield is caused by strong induction electron-withdrawing effect of the trifluoromethyl group in ortho-position to the amine group) of yellow crystalline solid, mp. 452–454 K. $^1$H NMR (CDCl$_3$): $\delta$ 7.31 (tt, $J_1$ = 7.4, 1.2 Hz, 1H), 7.48–7.63 (m, 6H), 8.13–8.19 (m, 4H), 8.95 (s, 1H); $^{13}$C NMR (CDCl$_3$): $\delta$ 116.9, 119.9, 122.7, 124.8, 125.4, 127.5, 129.0, 129.1, 129.3, 129.6 (q, $J_{CF} = 5.4$ Hz), 131.3, 132.2, 133.7, 139.8, 144.0, 144.5, 150.1. Single crystals suitable for X-ray diffraction were grown by slow evaporation from toluene solution.

S3. Refinement

As the structure contains only C, H, N and F atoms Friedel pairs were merged and absolute structure was not determined. H atoms were included into refinement in geometrically calculated positions, with C—H = 0.93 Å, and $U_{iso}(H) = 1.2 U_{eq}(C)$ for the aromatic CH groups, and constrained as a part of a riding model.

Figure 1
The best view of the molecule of title compound showing displacement ellipsoids at the 50% probability level.
Figure 2
Projection of the unit-cell contents along [010]. The mutual arrangement of the molecules forming π–π interactions is illustrated. The unit cell origin is at the lower left-hand corner of the cell with $b$ axis pointed down.
Figure 3
Projection of the unit-cell contents along [100] showing layered structure. The unit cell origin is at the lower right-hand corner of the cell with $a$ axis pointed down.

1,3-Diphenyl-8-trifluoromethyl-1H-pyrazolo[3,4-b]quinoline

Crystal data
C$_{23}$H$_{14}$F$_3$N$_3$
$M_r$ = 389.37
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 11.8299$ (5) Å
$b = 6.9788$ (3) Å
$c = 12.1306$ (4) Å
$\beta = 112.765$ (2)$^\circ$
$V = 923.47$ (6) Å$^3$
$Z = 2$

$F(000) = 400$
$D_x = 1.400$ Mg m$^{-3}$
Melting point = 452–454 K
Mo Ka radiation, $\lambda = 0.71073$ Å
Cell parameters from 2631 reflections
$\theta = 0.1–30.0^\circ$
$\mu = 0.11$ mm$^{-1}$
$T = 293$ K
Block, yellow
$0.27 \times 0.25 \times 0.20$ mm
Data collection
Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Horizontally mounted graphite crystal monochromator
Detector resolution: 9 pixels mm\(^{-1}\)
\(\omega\) scans
Absorption correction: multi-scan
\((\text{DENZO and SCALEPACK; Otwinowski \\& Minor, 1997})\)

Data collection statistics
\(T_{\text{min}} = 0.972, T_{\text{max}} = 0.979\)
4497 measured reflections
4497 independent reflections
2183 reflections with \(I > 2\sigma(I)\)
\(R_{\text{int}} = 0.018\)
\(\theta_{\text{max}} = 30.0^\circ, \theta_{\text{min}} = 3.1^\circ\)

Refinement
Refinement on \(F^2\)
Least-squares matrix: full
\(R[F^2 > 2\sigma(F^2)] = 0.044\)
\(wR(F^2) = 0.104\)
\(S = 1.05\)
2876 reflections
262 parameters
1 restraint
0 constraints

Refinement on \(F^2\)
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
\((\Delta/\sigma)_{\text{max}} < 0.001\)
\(\Delta \rho_{\text{max}} = 0.16\ \text{e} \cdot \text{Å}^{-3}\)
\(\Delta \rho_{\text{min}} = -0.18\ \text{e} \cdot \text{Å}^{-3}\)

Special details
Geometry. All e.s.d.'s 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.

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\(^2\))

| Atom | \(x\)      | \(y\)      | \(z\)      | \(U_{\text{eq}}/U_{\text{eq}}\) |
|------|-------------|-------------|-------------|----------------------------------|
| N1   | -0.18386 (15) | 0.2365 (4)  | 0.65903 (14) | 0.0473 (4)                       |
| N2   | -0.30046 (15) | 0.2283 (3)  | 0.57218 (15) | 0.0491 (4)                       |
| C3   | -0.29086 (18) | 0.2297 (4)  | 0.46736 (18) | 0.0454 (5)                       |
| C3A  | -0.16388 (17) | 0.2389 (4)  | 0.48271 (16) | 0.0422 (4)                       |
| C4   | -0.09599 (18) | 0.2371 (4)  | 0.41296 (17) | 0.0453 (5)                       |
| H4   | -0.1342      | 0.2327      | 0.3301      | 0.054*                           |
| C4A  | 0.03230 (18)  | 0.2421 (4)  | 0.46963 (16) | 0.0432 (4)                       |
| C5   | 0.1094 (2)   | 0.2426 (5)  | 0.40413 (18) | 0.0518 (5)                       |
| H5   | 0.0743       | 0.2407      | 0.3210      | 0.062*                           |
| C6   | 0.2333 (2)   | 0.2456 (5)  | 0.4611 (2)  | 0.0572 (6)                       |
| H6   | 0.2822       | 0.2441      | 0.4168      | 0.069*                           |
| C7   | 0.28812 (19) | 0.2510 (5)  | 0.5865 (2)  | 0.0535 (5)                       |
| H7   | 0.3731       | 0.2536      | 0.6242      | 0.064*                           |
| C8   | 0.21850 (18) | 0.2525 (4)  | 0.65379 (17) | 0.0455 (4)                       |
| C8A  | 0.08787 (17) | 0.2470 (4)  | 0.59753 (16) | 0.0410 (4)                       |
### Atomic displacement parameters (Å²)

|      | $U^{11}$  | $U^{22}$  | $U^{33}$  | $U^{12}$  | $U^{13}$  | $U^{23}$  |
|------|-----------|-----------|-----------|-----------|-----------|-----------|
| N1   | 0.0495 (9)| 0.0539 (11)| 0.0428 (8)| 0.0010 (12)| 0.0225 (7)| 0.0000 (11)|
| N2   | 0.0477 (9)| 0.0514 (11)| 0.0502 (9)| 0.0000 (11)| 0.0211 (7)| 0.0007 (11)|
| C3   | 0.0494 (10)| 0.0415 (12)| 0.0457 (10)| −0.0017 (12)| 0.0190 (8)| 0.0002 (11)|
| C3A  | 0.0477 (9)| 0.0385 (10)| 0.0405 (9)| −0.0031 (12)| 0.0172 (8)| −0.0024 (11)|
| C4   | 0.0548 (11)| 0.0457 (12)| 0.0362 (8)| −0.0032 (13)| 0.0183 (8)| −0.0025 (12)|
| C4A  | 0.0525 (10)| 0.0392 (10)| 0.0422 (9)| −0.0029 (12)| 0.0231 (8)| −0.0025 (11)|
| C5   | 0.0632 (12)| 0.0531 (13)| 0.0481 (10)| −0.0026 (16)| 0.0313 (10)| −0.0034 (15)|
| C6   | 0.0622 (13)| 0.0584 (15)| 0.0646 (13)| −0.0020 (17)| 0.0395 (11)| −0.0050 (17)|
| C7   | 0.0488 (10)| 0.0507 (13)| 0.0651 (12)| −0.0026 (14)| 0.0268 (10)| −0.0041 (15)|
| C8   | 0.0490 (10)| 0.0386 (10)| 0.0494 (10)| −0.0003 (12)| 0.0195 (8)| −0.0034 (12)|
| C8A  | 0.0496 (10)| 0.0335 (9)| 0.0436 (9)| 0.0001 (12)| 0.0220 (8)| −0.0022 (11)|
| N9   | 0.0489 (8)| 0.0445 (9)| 0.0388 (7)| −0.0008 (11)| 0.0191 (7)| −0.0026 (10)|
| C9A  | 0.0502 (10)| 0.0388 (10)| 0.0405 (9)| −0.0013 (12)| 0.0223 (8)| −0.0018 (12)|
| C11  | 0.0608 (11)| 0.0456 (11)| 0.0433 (9)| 0.0046 (14)| 0.0274 (9)| 0.0027 (13)|
| C12  | 0.0760 (16)| 0.0589 (16)| 0.0523 (13)| −0.0056 (14)| 0.0351 (12)| −0.0023 (12)|
| C13  | 0.095 (2)| 0.075 (2)| 0.0485 (13)| −0.0102 (17)| 0.0306 (14)| −0.0091 (14)|

*Estimated standard deviations in parentheses.*
### Geometric parameters (Å, °)

| Bond/Interatomic Distance | Value (Å) | Bond/Interatomic Distance | Value (Å) |
|---------------------------|-----------|---------------------------|-----------|
| N1—C9A                    | 1.376 (2) | C12—C13                   | 1.393 (3) |
| N1—N2                     | 1.375 (2) | C12—H12                   | 0.9300    |
| N1—C11                    | 1.427 (2) | C13—C14                   | 1.372 (4) |
| N2—C3                     | 1.320 (3) | C13—H13                   | 0.9300    |
| C3—C3A                    | 1.442 (3) | C14—C15                   | 1.361 (4) |
| C3—C31                    | 1.472 (3) | C14—H14                   | 0.9300    |
| C3A—C4                    | 1.374 (3) | C15—C16                   | 1.392 (4) |
| C3A—C9A                   | 1.429 (3) | C15—H15                   | 0.9300    |
| C4—C4A                    | 1.403 (3) | C16—H16                   | 0.9300    |
| C4—H4                     | 0.9300    | C31—C36                   | 1.378 (3) |
| C4A—C5                    | 1.422 (3) | C31—C32                   | 1.396 (3) |
| C4A—C8A                   | 1.432 (3) | C32—C33                   | 1.378 (4) |
| C5—C6                     | 1.358 (3) | C32—H32                   | 0.9300    |
| C5—H5                     | 0.9300    | C33—C34                   | 1.380 (5) |
| C6—C7                     | 1.404 (3) | C33—H33                   | 0.9300    |
| C6—H6                     | 0.9300    | C34—C35                   | 1.375 (4) |
| C7—C8                     | 1.366 (3) | C34—H34                   | 0.9300    |
| C7—H7                     | 0.9300    | C35—C36                   | 1.387 (3) |
| C8—C8A                    | 1.428 (3) | C35—H35                   | 0.9300    |
| C8—C80                    | 1.494 (3) | C36—H36                   | 0.9300    |
| C8A—N9                    | 1.360 (2) | C80—F83                   | 1.335 (3) |
| N9—C9A                    | 1.315 (2) | C80—F82                   | 1.343 (4) |
| C11—C12                   | 1.369 (3) | C80—F81                   | 1.343 (4) |
| C11—C16                   | 1.387 (3) |                           |           |
| N9—F82                    | 2.859 (3) | N9—C80                    | 2.808 (3) |
| N9—F81                    | 2.886 (2) |                           |           |

### Supporting Information

**C14** 0.106 (2) 0.084 (2) 0.0499 (12) 0.009 (2) 0.0448 (14) 0.0019 (17)  
**C15** 0.0898 (19) 0.092 (2) 0.0646 (16) −0.0012 (19) 0.0481 (16) 0.0157 (17)  
**C16** 0.0735 (16) 0.0687 (18) 0.0587 (14) −0.0023 (15) 0.0355 (13) 0.0074 (14)  
**C31** 0.0464 (10) 0.0454 (14) 0.0520 (11) 0.0004 (11) 0.0169 (9) −0.0019 (11)  
**C32** 0.0515 (12) 0.0652 (16) 0.0629 (14) −0.0039 (14) 0.0238 (11) −0.0039 (14)  
**C33** 0.0528 (14) 0.080 (2) 0.0799 (19) −0.0115 (16) 0.0221 (13) −0.0157 (18)  
**C34** 0.0588 (15) 0.093 (3) 0.0647 (16) −0.0047 (17) 0.0059 (12) −0.0165 (17)  
**C35** 0.0726 (16) 0.097 (3) 0.0521 (13) −0.003 (2) 0.0114 (12) 0.0035 (19)  
**C36** 0.0565 (12) 0.0682 (19) 0.0554 (13) −0.0052 (14) 0.0170 (10) 0.0059 (13)  
**C80** 0.0538 (12) 0.0606 (16) 0.0529 (11) 0.0031 (15) 0.0176 (10) −0.0045 (14)  
**F81** 0.0799 (12) 0.0745 (11) 0.0595 (10) 0.0008 (10) 0.0192 (9) −0.0227 (9)  
**F82** 0.0823 (12) 0.0769 (12) 0.0544 (9) 0.0061 (10) 0.0226 (9) 0.0131 (9)  
**F83** 0.0526 (7) 0.1111 (15) 0.0676 (8) −0.0001 (12) 0.0093 (6) −0.0062 (12)
sup-8

supporting information

N2—C3—C3A 110.47 (17)  C15—C14—C13 120.3 (2)
N2—C3—C31 120.29 (18)  C15—C14—H14 119.9
C3A—C3—C31 129.21 (18)  C13—C14—H14 119.9
C4—C3A—C9A 116.85 (17)  C14—C15—C16 121.0 (3)
C4—C3A—C3 138.44 (18)  C14—C15—H15 119.5
C9A—C3A—C3 104.65 (15)  C16—C15—H15 119.5
C3A—C4—C4A 118.50 (17)  C11—C16—C15 118.4 (3)
C3—C4—H4 120.8  C11—C16—H16 120.8
C4A—C4—H4 120.8  C15—C16—H16 120.8
C4—C4A—C5 122.12 (17)  C36—C31—C32 118.8 (2)
C4—C4A—C8A 119.17 (16)  C36—C31—C3 121.0 (2)
C5—C4A—C8A 118.71 (18)  C32—C31—C3 120.2 (2)
C6—C5—C4A 116.85 (17)  C33—C32—C31 120.1 (3)
C4A—C5—H5 119.5  C33—C32—H32 120.0
C4—C5—H5 119.5  C31—C32—H32 120.0
C5—C6—C7 120.43 (18)  C34—C33—C32 120.9 (3)
C5—C6—H6 119.8  C34—C33—H33 119.6
C7—C6—H6 119.8  C32—C33—H33 119.6
C8—C7—C6 121.0 (2)  C35—C34—C33 119.2 (3)
C8—C7—H7 119.5  C35—C34—H34 120.4
C6—C7—H7 119.5  C33—C34—H34 120.4
C7—C8—C8A 120.35 (19)  C34—C35—C36 120.3 (3)
C7—C8—C80 120.32 (19)  C34—C35—H35 119.8
C8A—C8—C80 119.32 (17)  C36—C35—H35 119.8
N9—C8A—C8 118.39 (17)  C31—C36—C35 120.7 (3)
N9—C8A—C4A 123.15 (17)  C31—C36—H36 119.6
C8—C8A—C4A 118.47 (16)  C35—C36—H36 119.6
C9A—N9—C8A 114.56 (16)  F83—C80—F82 106.0 (2)
N9—C9A—C80 126.14 (16)  F83—C80—F81 106.3 (2)
N9—C9A—C3A 127.78 (16)  F82—C80—F81 106.12 (18)
N1—C9A—C3A 106.07 (16)  F83—C80—C8 112.35 (18)
C12—C11—C16 121.0 (2)  F82—C80—C8 112.9 (2)
C12—C11—N1 120.6 (2)  F81—C80—C8 112.6 (2)
C16—C11—N1 118.3 (2)  C80—F81—N9 73.15 (13)
C11—C12—C13 119.4 (2)  C80—F82—N9 74.18 (13)
C11—C12—H12 120.3

C9A—N1—N2—C3 0.0 (3)  N2—N1—C9A—C3A 0.0 (3)
C11—N1—N2—C3 179.2 (3)  C11—N1—C9A—C3A −179.2 (3)
N1—N2—C3—C3A 0.1 (3)  C4—C3A—C9A—N9 0.7 (4)
N1—N2—C3—C31 178.3 (2)  C3—C3A—C9A—N9 178.4 (3)
N2—C3—C3A—C4 176.8 (3)  C4—C3A—C9A—N1 −177.6 (2)
C31—C3—C3A—C4 −1.2 (6)  C3—C3A—C9A—N1 0.1 (3)
N2—C3—C3A—C9A −0.1 (3)  C9A—N1—C11—C12 29.2 (4)
C31—C3—C3A—C9A −178.1 (3)  N2—N1—C11—C12 −149.9 (3)
C9A—C3A—C4—C4A −0.8 (4)  C9A—N1—C11—C16 −153.3 (3)
C3—C3A—C4—C4A −177.5 (3)  N2—N1—C11—C16 27.6 (4)
C3A—C4—C4A—C5 −179.4 (3)  C16—C11—C12—C13 −0.9 (4)
C3A—C4—C4A—C8A 0.6 (4) N1—C11—C12—C13 176.5 (3)
C4—C4A—C5—C6 −179.4 (3) C11—C12—C13—C14 −0.3 (5)
C8A—C4A—C5—C6 0.6 (5) C12—C13—C14—C15 1.4 (6)
C4A—C5—C6—C7 −0.9 (5) C13—C14—C15—C16 −1.2 (6)
C5—C6—C7—C8 0.3 (5) C12—C11—C16—C15 1.1 (4)
C6—C7—C8—C8A 0.5 (5) N1—C11—C16—C15 −176.3 (3)
C6—C7—C8—C80 −178.5 (3) C14—C15—C16—C11 0.0 (5)
C7—C8—C8A—N9 179.6 (3) N2—C3—C31—C36 157.4 (3)
C80—C8—C8A—N9 −1.4 (4) C3A—C3—C31—C36 −24.7 (4)
C8—C8A—C4A—C80 178.3 (3) C3A—C3—C31—C36 −23.9 (4)
C8—C8A—C4A—C80 178.3 (3) C3A—C3—C31—C36 −23.9 (4)
C4—C4A—C8A—N9 −0.2 (4) C36—C31—C32—C33 −0.3 (4)
C4—C4A—C8A—N9 −179.9 (3) C3—C31—C32—C33 −179.0 (3)
C4—C4A—C8A—C8 0.1 (4) C3—C31—C32—C33 −179.0 (3)
C5—C4A—C8A—C8 0.1 (4) C3—C31—C32—C33 −179.0 (3)
C8A—C8—C8A—C80 179.8 (3) C3—C31—C32—C33 −179.0 (3)
C8A—C8—C8A—N9 179.8 (3) C3—C31—C32—C33 −179.0 (3)
C4A—C8A—N9—C9A 0.1 (4) C3—C31—C32—C33 −179.0 (3)
C4A—C8A—N9—C9A 0.1 (4) C3—C31—C32—C33 −179.0 (3)
C8A—C8—C8A—N9 −0.2 (4) C3—C31—C32—C33 −179.0 (3)
C8A—C8—C8A—N9 −178.9 (3) C3—C31—C32—C33 −179.0 (3)
C4A—C8A—N9—C80 0.1 (4) C3—C31—C32—C33 −179.0 (3)
C4A—C8A—N9—C80 0.1 (4) C3—C31—C32—C33 −179.0 (3)
C8—C8A—N9—C80 −21.1 (2) C7—C8—C80—F82i 1.4 (4)
C4A—C8A—N9—C80 159.3 (2) C8A—C8—C80—F82 179.6 (3)
C8—C8A—N9—F81 23.3 (2) C7—C8—C80—F82 −121.3 (3)
C4A—C8A—N9—F81 23.3 (2) C7—C8—C80—F82 −121.3 (3)
C8A—N9—C9A—N1 177.7 (2) C7—C8—C80—F82 59.7 (3)
C8A—N9—C9A—C3A −0.3 (4) C8A—C8—C80—F81 −60.4 (3)
N2—N1—C9A—N9 −178.4 (3) C7—C8—C80—N9 179.7 (3)
C11—N1—C9A—N9 2.4 (5) C8A—C8—C80—N9 0.68 (19)

Hydrogen-bond geometry (Å, º)

| D—H···A | D—H | H···A | D···A | D—H···A |
|---------|------|-------|-------|---------|
| C12—H12···N9 | 0.93 | 2.50 | 3.042 (3) | 118 |
| C7—H7···F83 | 0.93 | 2.35 | 2.692 (3) | 102 |
| C36—H36···F82i | 0.93 | 2.56 | 3.357 (3) | 144 |
| C13—H13···Cg4ii | 0.93 | 2.92 | 3.729 (4) | 146 |
| C33—H33···Cg4ii | 0.93 | 3.03 | 3.697 (4) | 130 |

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