3-[(*E*)-4-(2-Nitrophenyl)vinyl]-1-(tri-fluoromethyl)-1,2,4-triazolo[4,3-*a*]-quinoxaline

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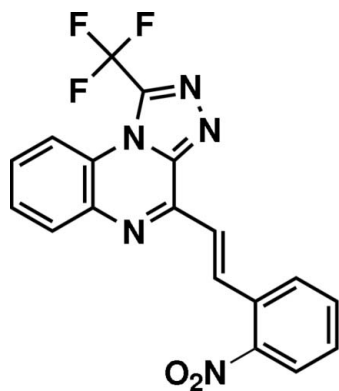Correspondence e-mail: athiru@vsnl.net

In the title molecule, $C_{18}H_{10}F_3N_5O_2$, the 1,2,4-triazolo[4,3-*a*]-quinoxaline unit is nearly planar. The central pyrazine ring makes dihedral angles of 1.67 (6) and 2.44 (5)° with the 1,2,4-triazole and fused benzene ring, respectively. The nitrophenyl ring makes dihedral angles of 2.82 (6), 3.15 (6) and 3.63 (6)° with the triazole, pyrazine and benzene rings, respectively. The nitro group is slightly twisted away from the plane of the attached benzene ring. C—H⋯O and C—H⋯F hydrogen bonds are found in the crystal structure.

Related literature

For the uses of [1,2,4]triazoloquinoxalines, see Ali *et al.* (2004); Bicking (1959); Chimirri *et al.* (2002); Dawood *et al.* (2006); Ilkay *et al.* (2004); Potts (1961); Trivedi (1988); Xie *et al.* (2005).

Experimental

Crystal data

$C_{18}H_{10}F_3N_5O_2$	$V = 1624.86$ (7) Å³
$M_r = 385.31$	$Z = 4$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 8.0065$ (2) Å	$\mu = 0.13$ mm⁻¹
$b = 16.9010$ (4) Å	$T = 200$ (2) K
$c = 12.0204$ (3) Å	$0.37 \times 0.35 \times 0.22$ mm
$\beta = 92.633$ (2)°	

Data collection

Oxford Diffraction Gemini diffractometer	$T_{min} = 0.899$, $T_{max} = 1.000$ (expected range = 0.874–0.972)
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)	15678 measured reflections
	5345 independent reflections
	3157 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.023$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$	253 parameters
$wR(F^2) = 0.125$	H-atom parameters constrained
$S = 0.98$	$\Delta\rho_{max} = 0.35$ e Å⁻³
5345 reflections	$\Delta\rho_{min} = -0.28$ e Å⁻³

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C2—H2⋯O1	0.95	2.30	2.7633 (15)	109
C5A—H5⋯O2ⁱ	0.95	2.56	3.2875 (16)	134
C8—H8⋯F1	0.95	2.43	3.1362 (15)	131
C8—H8⋯F2	0.95	2.47	3.2139 (15)	135
C14—H14⋯O1ⁱⁱ	0.95	2.59	3.4551 (17)	151
C16—H16⋯F3ⁱⁱⁱ	0.95	2.55	3.2850 (16)	135

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2003).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CS2062).

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supplementary materials

3-[(*E*)-4-(2-Nitrophenyl)vinyl]-1-(trifluoromethyl)-1,2,4-triazolo[4,3-*a*]quinoxaline

A. Thiruvalluvar, M. Subramanyam, R. J. Butcher, S. Wagle and **A. V. Adhikari**

Comment

In addition to purines and pteridines, many other fused heterocyclic ring systems are known. Of these the most important is that containing ring junction nitrogen, in which the nitrogen is common to two rings. The vast majority of these systems do not occur naturally, they have been the subject of many studies from the theoretical viewpoint and for the preparation of biologically active analogues. Earlier studies revealed that most of the compounds derived from 1,2,4-triazoles have been shown to display a wide spectrum of biological activities. Moreover, a few fused triazoles of different heterocycles have been found to be significant anticonvulsant and tranquillizing agents. Also, 1,2,4-triazolo quinoxalines have been reported as antidepressant, cardiotonics and antifatigue agents (Ali *et al.*, 2004; Bicking, 1959; Chimirri *et al.*, 2002; Dawood *et al.*, 2006; Ilkay *et al.*, 2004; Potts, 1961; Trivedi, 1988; Xie *et al.*, 2005).

In the title molecule, $C_{18}H_{10}F_3N_5O_2$, Fig.1, the [1,2,4]triazolo[4,3-*a*]quinoxaline unit is nearly planar. The central pyrazine ring makes a dihedral angle of 1.67 (6)° and 2.44 (5)° with that of the 1,2,4-triazole and the fused benzene ring respectively. The nitro phenyl ring makes a dihedral angle of 2.82 (6)°, 3.15 (6)°, and 3.63 (6)° with that of triazole, pyrazine and benzene rings respectively. The nitro group is slightly twisted away from the plane of the attached phenyl ring. C—H⋯O and C—H⋯F hydrogen bonds are found in the crystal structure; see Fig. 2., and the hydrogen bond table.

Experimental

To a mixture of compounds 4-methyl-1-(trifluoromethyl)[1,2,4]triazolo[4,3-*a*]quinoxaline (5.0 g, 0.0198 mol), and 2-nitrobenzaldehyde (3.14 g, 0.0208 mol) in methanol (20 ml) added catalytic amount (0.2 ml) of conc. sulfuric acid. The reaction mass was refluxed (338 K) for 8 h. The reaction mass was cooled to room temperature, and kept overnight. The separated solid was filtered, washed with methanol (5 ml) to obtain the title compound. The compound was further recrystalized from ethanol to give pale yellow crystals 4.0 g, 52.6%.

Refinement

H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.95 Å and U_{iso} = 1.2 times $U_{eq}(C)$.
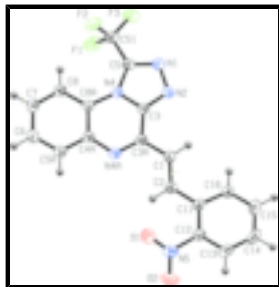
supplementary materials

Figures

Fig. 1. The molecular structure of the title compound, showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radius.
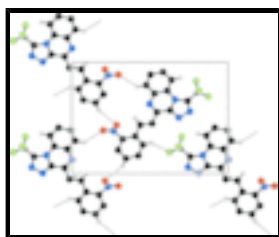

Fig. 2. The packing of the title compound, viewed down the *a* axis. Dashed lines indicate hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted.

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Crystal data

$C_{18}H_{10}F_3N_5O_2$	$F_{000} = 784$
$M_r = 385.31$	$D_x = 1.575$ Mg m^{-3}
Monoclinic, $P2_1/n$	Melting point: 472(1) K
Hall symbol: -P 2yn	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.0065$ (2) Å	Cell parameters from 6025 reflections
$b = 16.9010$ (4) Å	$\theta = 4.8–32.5º$
$c = 12.0204$ (3) Å	$\mu = 0.13$ mm^{-1}
$\beta = 92.633$ (2)º	$T = 200$ (2) K
$V = 1624.86$ (7) Å^3	Prism, pale yellow
$Z = 4$	$0.37 \times 0.35 \times 0.22$ mm

Data collection

Oxford Diffraction Gemini diffractometer	5345 independent reflections
Radiation source: fine-focus sealed tube	3157 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.023$
$T = 200(2)$ K	$\theta_{max} = 32.6º$
φ and ω scans	$\theta_{min} = 4.8º$
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)	$h = -11 \rightarrow 11$
$T_{min} = 0.899$, $T_{max} = 1.000$	$k = -25 \rightarrow 25$
15678 measured reflections	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.043$	H-atom parameters constrained
$wR(F^2) = 0.125$	$w = 1/[\sigma^2(F_o^2) + (0.0729P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.98$	$(\Delta/\sigma)_{max} = 0.001$
5345 reflections	$\Delta\rho_{max} = 0.35$ e Å^{-3}
253 parameters	$\Delta\rho_{min} = -0.28$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	$U_{iso}*/U_{eq}$
F1	0.33806 (11)	0.79608 (5)	0.83090 (7)	0.0536 (3)
F2	0.56207 (10)	0.81556 (5)	0.74471 (7)	0.0473 (3)
F3	0.33485 (13)	0.87452 (5)	0.69060 (8)	0.0638 (4)
O1	0.30844 (12)	0.28804 (5)	0.43450 (8)	0.0420 (3)
O2	0.12053 (14)	0.20138 (6)	0.38762 (11)	0.0588 (4)
N1	0.26886 (14)	0.75604 (6)	0.55632 (9)	0.0381 (3)
N2	0.23975 (14)	0.68574 (6)	0.50247 (9)	0.0359 (3)
N4	0.37684 (11)	0.66121 (6)	0.66443 (7)	0.0253 (3)
N4A	0.37242 (12)	0.49810 (6)	0.62414 (8)	0.0293 (3)
N5	0.17977 (14)	0.26776 (6)	0.38229 (9)	0.0367 (3)
C1	0.22162 (15)	0.51486 (7)	0.44843 (10)	0.0302 (3)
C2	0.17674 (14)	0.43913 (7)	0.43653 (9)	0.0290 (3)
C3	0.30453 (14)	0.63014 (7)	0.56780 (9)	0.0268 (3)
C3A	0.30274 (14)	0.54560 (7)	0.55073 (9)	0.0274 (3)
C4A	0.45134 (14)	0.52974 (7)	0.71888 (9)	0.0266 (3)
C5	0.34938 (15)	0.74113 (7)	0.65139 (10)	0.0305 (3)
C5A	0.53147 (15)	0.47701 (7)	0.79337 (10)	0.0329 (3)
C6	0.61637 (17)	0.50386 (8)	0.88796 (11)	0.0384 (4)
C7	0.62241 (16)	0.58451 (8)	0.91106 (10)	0.0373 (4)
C8	0.54455 (15)	0.63835 (7)	0.84044 (10)	0.0314 (3)
C8A	0.45896 (14)	0.61160 (7)	0.74388 (9)	0.0254 (3)
C11	0.09609 (14)	0.40639 (7)	0.33468 (9)	0.0283 (3)
C12	0.09491 (15)	0.32572 (7)	0.30827 (10)	0.0298 (3)
C13	0.01979 (17)	0.29588 (8)	0.21091 (12)	0.0400 (4)
C14	−0.05853 (17)	0.34677 (9)	0.13569 (11)	0.0447 (5)
C15	−0.06427 (16)	0.42677 (9)	0.16040 (11)	0.0416 (4)
C16	0.01072 (16)	0.45550 (8)	0.25819 (10)	0.0342 (4)
C51	0.39666 (17)	0.80652 (7)	0.72976 (12)	0.0389 (4)
H1	0.19990	0.55012	0.38794	0.0362*
H2	0.19835	0.40442	0.49767	0.0348*

H5	0.52718	0.42184	0.77840	0.0395*
H6	0.67091	0.46736	0.93754	0.0460*
H7	0.68122	0.60262	0.97662	0.0448*
H8	0.54894	0.69326	0.85719	0.0377*
H13	0.02229	0.24068	0.19614	0.0479*
H14	−0.10796	0.32725	0.06776	0.0536*
H15	−0.12013	0.46215	0.10981	0.0499*
H16	0.00385	0.51049	0.27373	0.0410*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0648 (5)	0.0496 (5)	0.0472 (5)	−0.0069 (4)	0.0121 (4)	−0.0219 (4)
F2	0.0486 (5)	0.0391 (4)	0.0534 (5)	−0.0125 (4)	−0.0049 (4)	−0.0113 (4)
F3	0.0897 (7)	0.0208 (4)	0.0781 (7)	0.0094 (4)	−0.0264 (5)	−0.0086 (4)
O1	0.0420 (5)	0.0355 (5)	0.0478 (5)	0.0043 (4)	−0.0047 (4)	0.0018 (4)
O2	0.0655 (7)	0.0227 (5)	0.0879 (9)	−0.0070 (5)	0.0008 (6)	0.0064 (5)
N1	0.0484 (6)	0.0241 (5)	0.0409 (6)	−0.0006 (5)	−0.0084 (5)	0.0002 (5)
N2	0.0488 (6)	0.0237 (5)	0.0341 (6)	−0.0012 (5)	−0.0103 (5)	0.0006 (4)
N4	0.0307 (5)	0.0203 (4)	0.0247 (5)	−0.0019 (4)	−0.0022 (4)	−0.0026 (4)
N4A	0.0371 (5)	0.0229 (5)	0.0274 (5)	−0.0029 (4)	−0.0027 (4)	−0.0029 (4)
N5	0.0404 (6)	0.0237 (5)	0.0463 (6)	0.0003 (5)	0.0047 (5)	−0.0019 (5)
C1	0.0384 (6)	0.0245 (6)	0.0271 (6)	−0.0013 (5)	−0.0054 (5)	−0.0024 (5)
C2	0.0333 (6)	0.0246 (6)	0.0286 (6)	0.0011 (5)	−0.0041 (5)	−0.0025 (5)
C3	0.0325 (6)	0.0231 (5)	0.0245 (5)	−0.0032 (4)	−0.0025 (4)	−0.0025 (4)
C3A	0.0336 (6)	0.0229 (5)	0.0254 (5)	−0.0038 (5)	−0.0008 (4)	−0.0032 (5)
C4A	0.0302 (6)	0.0232 (5)	0.0262 (5)	−0.0029 (4)	−0.0012 (4)	−0.0018 (5)
C5	0.0371 (6)	0.0191 (5)	0.0350 (6)	−0.0008 (5)	−0.0021 (5)	−0.0028 (5)
C5A	0.0407 (7)	0.0224 (5)	0.0352 (6)	−0.0005 (5)	−0.0039 (5)	0.0015 (5)
C6	0.0456 (7)	0.0337 (7)	0.0348 (7)	−0.0012 (6)	−0.0089 (5)	0.0066 (6)
C7	0.0450 (7)	0.0357 (7)	0.0303 (6)	−0.0068 (6)	−0.0088 (5)	−0.0007 (6)
C8	0.0406 (6)	0.0258 (6)	0.0274 (6)	−0.0054 (5)	−0.0026 (5)	−0.0033 (5)
C8A	0.0282 (5)	0.0225 (5)	0.0254 (5)	−0.0011 (4)	−0.0008 (4)	0.0007 (4)
C11	0.0308 (5)	0.0238 (5)	0.0298 (6)	−0.0033 (5)	−0.0031 (4)	−0.0040 (5)
C12	0.0294 (5)	0.0249 (5)	0.0348 (6)	−0.0022 (5)	0.0000 (5)	−0.0037 (5)
C13	0.0411 (7)	0.0326 (7)	0.0461 (8)	−0.0078 (6)	0.0007 (6)	−0.0147 (6)
C14	0.0470 (8)	0.0505 (9)	0.0356 (7)	−0.0107 (7)	−0.0093 (6)	−0.0149 (7)
C15	0.0406 (7)	0.0480 (8)	0.0350 (7)	−0.0018 (6)	−0.0114 (5)	−0.0014 (6)
C16	0.0386 (7)	0.0266 (6)	0.0364 (6)	−0.0002 (5)	−0.0094 (5)	−0.0015 (5)
C51	0.0478 (8)	0.0216 (6)	0.0465 (8)	−0.0012 (5)	−0.0051 (6)	−0.0048 (6)

Geometric parameters (Å, °)

F1—C51	1.3348 (17)	C5A—C6	1.3747 (18)
F2—C51	1.3370 (16)	C6—C7	1.3915 (19)
F3—C51	1.3289 (15)	C7—C8	1.3743 (18)
O1—N5	1.2301 (15)	C8—C8A	1.3958 (16)
O2—N5	1.2209 (15)	C11—C12	1.3998 (17)
N1—N2	1.3679 (15)	C11—C16	1.3942 (17)

N1—C5	1.3105 (16)	C12—C13	1.3860 (19)
N2—C3	1.3158 (16)	C13—C14	1.378 (2)
N4—C3	1.3778 (14)	C14—C15	1.386 (2)
N4—C5	1.3763 (16)	C15—C16	1.3832 (18)
N4—C8A	1.4106 (14)	C1—H1	0.9500
N4A—C3A	1.2997 (15)	C2—H2	0.9500
N4A—C4A	1.3842 (15)	C5A—H5	0.9500
N5—C12	1.4688 (16)	C6—H6	0.9500
C1—C2	1.3353 (17)	C7—H7	0.9500
C1—C3A	1.4596 (16)	C8—H8	0.9500
C2—C11	1.4661 (16)	C13—H13	0.9500
C3—C3A	1.4435 (17)	C14—H14	0.9500
C4A—C5A	1.3981 (16)	C15—H15	0.9500
C4A—C8A	1.4165 (17)	C16—H16	0.9500
C5—C51	1.4898 (18)		
F1···N4	3.0583 (13)	C3A···C16^i	3.4791 (17)
F1···C8	3.1362 (15)	C4A···C1^{iii}	3.4573 (16)
F1···C13^i	3.2779 (16)	C4A···C15^i	3.5586 (17)
F1···O1^{ii}	3.1065 (13)	C5···O1^{iii}	3.0124 (15)
F1···C14^i	3.3289 (17)	C5···C13^i	3.5096 (18)
F2···O2^{iii}	3.0727 (14)	C5A···O2^{viii}	3.2875 (16)
F2···C8	3.2139 (15)	C5A···C1^{iii}	3.5921 (17)
F2···N4	3.1312 (13)	C6···C16^{iii}	3.5992 (19)
F2···N5^{iii}	2.9792 (14)	C6···C6^{ix}	3.3475 (19)
F2···O1^{iii}	2.9977 (12)	C6···C7^{ix}	3.4852 (18)
F3···C16^{iv}	3.2850 (16)	C7···C6^{ix}	3.4852 (18)
F3···N1	2.6107 (14)	C7···N1^{iv}	3.3909 (17)
F1···H8	2.4300	C8···F1	3.1362 (15)
F1···H2^{ii}	2.7800	C8···C51	3.3325 (17)
F2···H8	2.4700	C8···C12^{iii}	3.5173 (17)
F3···H7^v	2.8300	C8···F2	3.2139 (15)
F3···H16^{iv}	2.5500	C8A···C15^i	3.4734 (17)
O1···C2	2.7633 (15)	C8A···O1^{iii}	3.3630 (15)
O1···N4^{iii}	2.9622 (13)	C11···C3^i	3.5198 (16)
O1···F1^{vi}	3.1065 (13)	C12···C8^{iii}	3.5173 (17)
O1···F2^{iii}	2.9977 (12)	C13···C5^i	3.5096 (18)
O1···C8A^{iii}	3.3630 (15)	C13···F1^i	3.2779 (16)
O1···C3^{iii}	3.3946 (15)	C14···F1^i	3.3289 (17)
O1···C5^{iii}	3.0124 (15)	C15···C8A^i	3.4734 (17)
O2···F2^{iii}	3.0727 (14)	C15···C4A^i	3.5586 (17)
O2···C5A^{vii}	3.2875 (16)	C16···C3A^i	3.4791 (17)
O1···H2	2.3000	C16···C6^{iii}	3.5992 (19)
O1···H14^{viii}	2.5900	C16···F3^v	3.2850 (16)

O2···H13	2.4900	C51···C8	3.3325 (17)
O2···H5^{vii}	2.5600	C1···H16	2.6700
N1···F3	2.6107 (14)	C5···H8	2.9900
N1···N4	2.2140 (14)	C16···H1	2.6600
N1···C7^{v}	3.3909 (17)	C51···H8	2.7100
N2···N4	2.2295 (14)	H1···N2	2.6900
N4···O1^{iii}	2.9622 (13)	H1···C16	2.6600
N4···N1	2.2140 (14)	H1···H16	2.1400
N4···F1	3.0583 (13)	H2···O1	2.3000
N4···F2	3.1312 (13)	H2···N4A	2.5600
N4···N4A	2.7989 (14)	H2···N5	2.6900
N4A···N4	2.7989 (14)	H2···F1^{vi}	2.7800
N4A···C1^{iii}	3.4109 (15)	H5···O2^{viii}	2.5600
N5···F2^{iii}	2.9792 (14)	H7···F3^{iv}	2.8300
N1···H7^{v}	2.6600	H7···N1^{iv}	2.6600
N2···H1	2.6900	H8···F1	2.4300
N4A···H2	2.5600	H8···F2	2.4700
N5···H2	2.6900	H8···C5	2.9900
C1···C5A^{iii}	3.5921 (17)	H8···C51	2.7100
C1···N4A^{iii}	3.4109 (15)	H13···O2	2.4900
C1···C4A^{iii}	3.4573 (16)	H14···O1^{vii}	2.5900
C2···O1	2.7633 (15)	H16···C1	2.6700
C3···C11^{i}	3.5198 (16)	H16···H1	2.1400
C3···O1^{iii}	3.3946 (15)	H16···F3^{v}	2.5500
N2—N1—C5	108.18 (10)	N5—C12—C11	120.94 (10)
N1—N2—C3	106.50 (10)	N5—C12—C13	116.07 (11)
C3—N4—C5	102.67 (9)	C11—C12—C13	122.96 (11)
C3—N4—C8A	120.60 (10)	C12—C13—C14	119.59 (12)
C5—N4—C8A	136.68 (10)	C13—C14—C15	119.15 (13)
C3A—N4A—C4A	119.04 (10)	C14—C15—C16	120.49 (13)
O1—N5—O2	123.20 (11)	C11—C16—C15	122.14 (12)
O1—N5—C12	118.46 (10)	F1—C51—F2	106.27 (11)
O2—N5—C12	118.34 (11)	F1—C51—F3	107.23 (11)
C2—C1—C3A	122.59 (11)	F1—C51—C5	112.84 (10)
C1—C2—C11	123.87 (11)	F2—C51—F3	107.41 (10)
N2—C3—N4	111.70 (10)	F2—C51—C5	113.02 (11)
N2—C3—C3A	128.39 (10)	F3—C51—C5	109.75 (11)
N4—C3—C3A	119.88 (10)	C2—C1—H1	119.00
N4A—C3A—C1	120.84 (11)	C3A—C1—H1	119.00
N4A—C3A—C3	120.92 (10)	C1—C2—H2	118.00
C1—C3A—C3	118.24 (10)	C11—C2—H2	118.00
N4A—C4A—C5A	117.35 (10)	C4A—C5A—H5	120.00
N4A—C4A—C8A	124.43 (10)	C6—C5A—H5	120.00
C5A—C4A—C8A	118.21 (10)	C5A—C6—H6	120.00
N1—C5—N4	110.96 (10)	C7—C6—H6	120.00
N1—C5—C51	120.62 (11)	C6—C7—H7	120.00

N4—C5—C51	128.42 (11)	C8—C7—H7	120.00
C4A—C5A—C6	120.94 (11)	C7—C8—H8	120.00
C5A—C6—C7	119.98 (12)	C8A—C8—H8	120.00
C6—C7—C8	120.98 (12)	C12—C13—H13	120.00
C7—C8—C8A	119.38 (11)	C14—C13—H13	120.00
N4—C8A—C4A	115.01 (10)	C13—C14—H14	120.00
N4—C8A—C8	124.49 (11)	C15—C14—H14	120.00
C4A—C8A—C8	120.50 (10)	C14—C15—H15	120.00
C2—C11—C12	123.72 (10)	C16—C15—H15	120.00
C2—C11—C16	120.65 (11)	C11—C16—H16	119.00
C12—C11—C16	115.61 (11)	C15—C16—H16	119.00
C5—N1—N2—C3	0.00 (15)	N2—C3—C3A—C1	0.73 (18)
N2—N1—C5—N4	0.03 (14)	N4—C3—C3A—N4A	−1.80 (17)
N2—N1—C5—C51	−179.10 (11)	N4—C3—C3A—C1	178.63 (10)
N1—N2—C3—N4	−0.06 (14)	N4A—C4A—C5A—C6	178.31 (11)
N1—N2—C3—C3A	177.98 (11)	C8A—C4A—C5A—C6	−0.44 (18)
C5—N4—C3—N2	0.08 (13)	N4A—C4A—C8A—N4	0.71 (16)
C5—N4—C3—C3A	−178.15 (10)	N4A—C4A—C8A—C8	−178.61 (11)
C8A—N4—C3—N2	−177.62 (10)	C5A—C4A—C8A—N4	179.36 (10)
C8A—N4—C3—C3A	4.16 (15)	C5A—C4A—C8A—C8	0.04 (17)
C3—N4—C5—N1	−0.07 (13)	N1—C5—C51—F1	123.92 (13)
C3—N4—C5—C51	178.98 (12)	N1—C5—C51—F2	−115.47 (13)
C8A—N4—C5—N1	177.04 (12)	N1—C5—C51—F3	4.40 (17)
C8A—N4—C5—C51	−3.9 (2)	N4—C5—C51—F1	−55.05 (17)
C3—N4—C8A—C4A	−3.52 (15)	N4—C5—C51—F2	65.57 (17)
C3—N4—C8A—C8	175.77 (11)	N4—C5—C51—F3	−174.56 (11)
C5—N4—C8A—C4A	179.76 (12)	C4A—C5A—C6—C7	0.45 (19)
C5—N4—C8A—C8	−1.0 (2)	C5A—C6—C7—C8	−0.1 (2)
C4A—N4A—C3A—C1	178.55 (10)	C6—C7—C8—C8A	−0.33 (19)
C4A—N4A—C3A—C3	−1.01 (16)	C7—C8—C8A—N4	−178.92 (11)
C3A—N4A—C4A—C5A	−177.11 (11)	C7—C8—C8A—C4A	0.34 (17)
C3A—N4A—C4A—C8A	1.56 (17)	C2—C11—C12—N5	−1.24 (18)
O1—N5—C12—C11	−33.51 (17)	C2—C11—C12—C13	−179.18 (12)
O1—N5—C12—C13	144.57 (12)	C16—C11—C12—N5	−179.76 (11)
O2—N5—C12—C11	147.64 (12)	C16—C11—C12—C13	2.30 (18)
O2—N5—C12—C13	−34.28 (17)	C2—C11—C16—C15	178.86 (11)
C3A—C1—C2—C11	−179.60 (11)	C12—C11—C16—C15	−2.57 (18)
C2—C1—C3A—N4A	17.38 (18)	N5—C12—C13—C14	−178.28 (12)
C2—C1—C3A—C3	−163.05 (11)	C11—C12—C13—C14	−0.2 (2)
C1—C2—C11—C12	159.64 (12)	C12—C13—C14—C15	−1.7 (2)
C1—C2—C11—C16	−21.91 (18)	C13—C14—C15—C16	1.4 (2)
N2—C3—C3A—N4A	−179.70 (12)	C14—C15—C16—C11	0.8 (2)

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) −*x*+1/2, *y*+1/2, −*z*+3/2; (iii) −*x*+1, −*y*+1, −*z*+1; (iv) *x*+1/2, −*y*+3/2, *z*+1/2; (v) *x*−1/2, −*y*+3/2, *z*−1/2; (vi) −*x*+1/2, *y*−1/2, −*z*+3/2; (vii) *x*−1/2, −*y*+1/2, *z*−1/2; (viii) *x*+1/2, −*y*+1/2, *z*+1/2; (ix) −*x*+1, −*y*+1, −*z*+2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O1	0.95	2.30	2.7633 (15)	109

C5A—H5···O2[viii]	0.95	2.56	3.2875 (16)	134
C8—H8···F1	0.95	2.43	3.1362 (15)	131
C8—H8···F2	0.95	2.47	3.2139 (15)	135
C14—H14···O1[vii]	0.95	2.59	3.4551 (17)	151
C16—H16···F3[v]	0.95	2.55	3.2850 (16)	135

Symmetry codes: (viii) $x+1/2$, $-y+1/2$, $z+1/2$; (vii) $x-1/2$, $-y+1/2$, $z-1/2$; (v) $x-1/2$, $-y+3/2$, $z-1/2$.
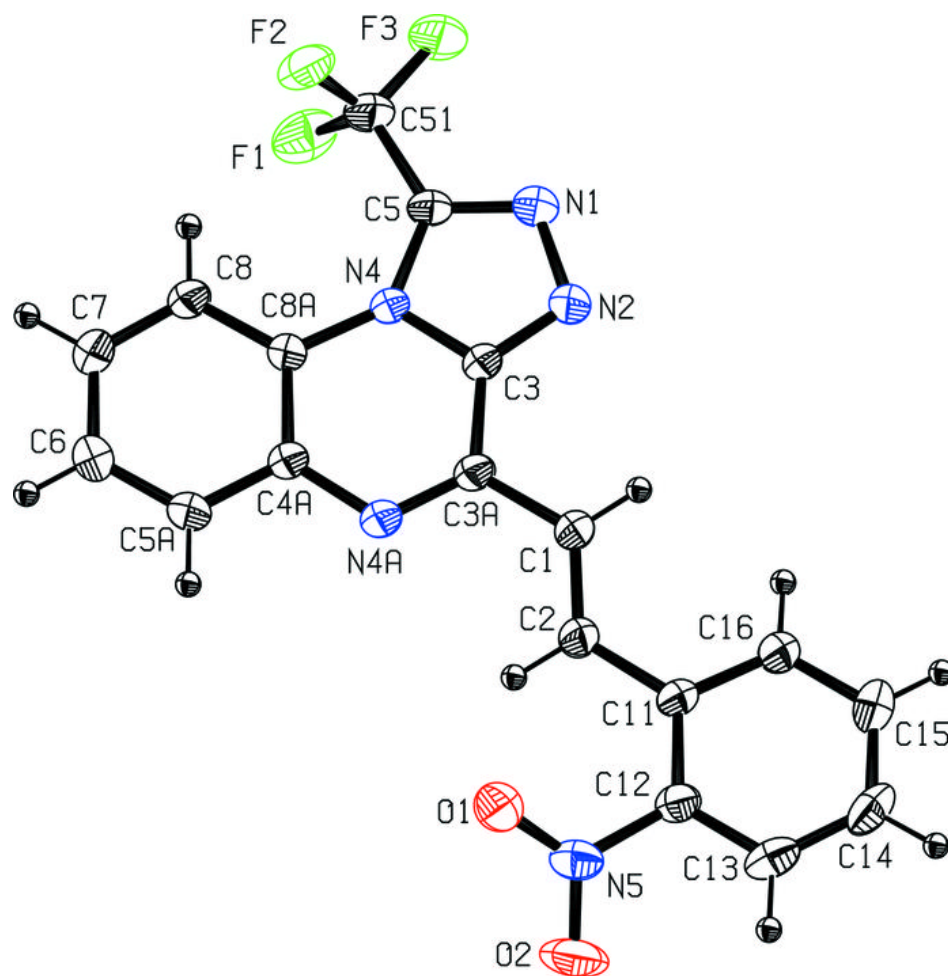
Fig. 1

Fig. 2