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(*E*)-4-Methoxy-*N*′-(2,4,5-trifluorobenzylidene)-benzohydrazide monohydrate

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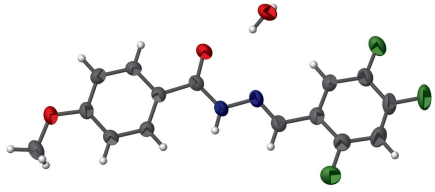
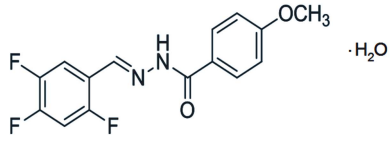
The title Schiff base compound, $C_{15}H_{11}F_3N_2O_2\cdot H_2O$, crystallized as a monohydrate. The conformation about the C=N bond is *E*. The molecule is almost planar, with the dihedral angle between the planes of the methoxybenzene and trifluorobenzylidene rings being 7.46 (6)°. In the crystal, molecules are linked by bifurcated O_{water}—H···(O,N) hydrogen bonds and N—H···O_{water} and O_{water}—H···O and C—H···O hydrogen bonds, forming chains along [100]. The chains are linked by C—H···O_{water} hydrogen bonds, forming slabs parallel to the *bc* plane. Within the slabs there are offset π–π interactions present [intercentroid distance = 3.7883 (7) Å].

3D view



Chemical scheme



Structure description

Benzohydrazide Schiff base compounds exhibit a wide range of biological activities and act as a promising lead compounds for the design of more efficient drugs (Negi *et al.*, 2012). Recently, benzohydrazones have attracted attention due to their versatile applications in various fields such as biology (Ibrahim *et al.*, 2016), medicine (Velezheva *et al.*, 2016) and catalysis (Selvamurugan *et al.*, 2016). These derivatives also exhibit antimicrobial (Pieczonka *et al.*, 2013), anti-proliferative (Yadagiri *et al.*, 2014) and antiplatelet (Mashayekhi *et al.*, 2013) activities.

The geometric parameters of the title molecule (Fig. 1) agree well with those reported for similar structures (Maheswari *et al.*, 2016; Nair *et al.*, 2012). The conformation about the C7=N1 bond is *E*. The dihedral angle between methoxyphenyl ring and trifluorobenzylidene ring is 7.46 (6)°.

In the crystal, molecules are linked by bifurcated O_{water}—H···(O,N) hydrogen bonds and N—H···O_{water} and O_{water}—H···O and C—H···O hydrogen bonds, forming chains

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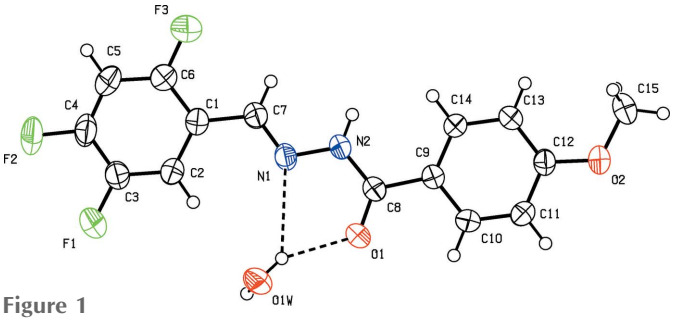

Figure 1
The molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 30% probability level. The bifurcated O_{water}—H···(O,N) hydrogen bonds are shown as dashed lines (see Table 1).

along [100]; see Table 1 and Fig. 2. The chains are linked by C—H···O_{water} hydrogen bonds, forming slabs parallel to the *bc* plane (Table 1 and Fig. 3). Within the slabs, there are offset π–π interactions present [$Cg1\cdots Cg2^{i}$ = 3. 7883 (3) Å,, interplanar distance = 3.5156 (6) Å, slippage = 1.746 Å; *Cg*1 and *Cg*2 are the centroids of rings C1–C6 and C9–C14, respectively; symmetry code: (i) $-x+1, -y-1, -z+1$].

Synthesis and crystallization

To mixture of 4-methoxybenzohydrazide (1.6 g, 0.01 mol) and 2,4,5-trifluorobenzaldehyde (1.6 ml, 0.01 mol) in ethanol (10 ml) were added a few drops of concentrated HCl. The reaction mixture was stirred for 30 min at room temperature. The insoluble solid that gradually formed was filtered and washed with petroleum ether and dried in a vacuum desiccator. The crude solid was recrystallized from DMSO solution, giving colourless block-like crystals (yield 96%).

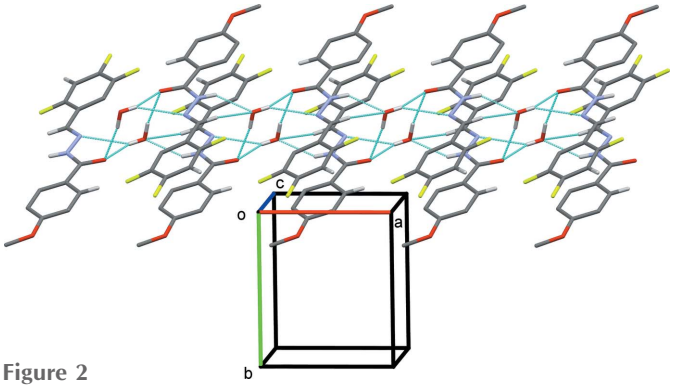

Figure 2
A partial view along the *c* axis of the crystal packing of the title compound. The hydrogen bonds (see Table 1) are shown as dashed lines and, for clarity, only the H atoms involved in these interactions are included.

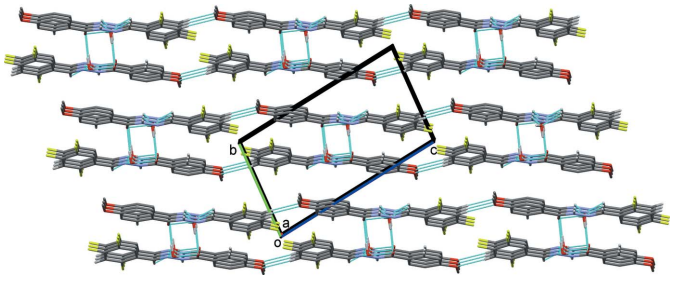

Figure 3
A view along the *a* axis of the crystal packing of the title compound. The hydrogen bonds (see Table 1) are shown as dashed lines and, for clarity, only the H atoms involved in these interactions are included.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O1	0.85 (2)	2.05 (2)	2.8376 (13)	154 (2)
O1*W*—H1*WA*···N1	0.85 (2)	2.61 (2)	3.2777 (14)	137 (2)
N2—H2···O1*W*^{i}	0.86	2.12	2.8681 (14)	145
O1*W*—H1*WB*···O1^{ii}	0.86 (2)	2.01 (2)	2.8635 (16)	170 (2)
C5—H5···O2^{iii}	0.93	2.49	3.4128 (15)	172
C7—H7···O1*W*^{i}	0.93	2.54	3.2191 (15)	130

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{11}F_3N_2O_2\cdot H_2O$
M_r	326.27
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, *b*, *c* (Å)	6.6872 (2), 7.9309 (2), 13.9723 (4)
α, β, γ (°)	82.348 (2), 84.783 (1), 88.710 (1)
V (Å^3)	731.35 (4)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	0.13
Crystal size (mm)	0.19 × 0.16 × 0.11
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.976, 0.986
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10841, 3036, 2559
R_{int}	0.023
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.629
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.036, 0.111, 1.04
No. of reflections	3036
No. of parameters	218
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.16, −0.20

Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008).

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x160846 [doi:10.1107/S2414314616008464]

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Crystal data

$C_{15}H_{11}F_3N_2O_2·H_2O$
M_r = 326.27
Triclinic, $P\overline{1}$
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c = 13.9723 (4) Å
α = 82.348 (2)°
β = 84.783 (1)°
γ = 88.710 (1)°
V = 731.35 (4) Å^3
Z = 2
F(000) = 336
D_x = 1.482 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3036 reflections
θ = 1.5–26.6°
μ = 0.13 mm^{-1}
T = 296 K
Block, colourless
0.19 × 0.16 × 0.11 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 0 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.976, T_{max} = 0.986
10841 measured reflections
3036 independent reflections
2559 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 26.6°, θ_{min} = 1.5°
h = −8→8
k = −9→9
l = −17→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.111
S = 1.04
3036 reflections
218 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0587P)^2 + 0.1124P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.105 (7)

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

	x	y	z	U_{iso}*/U_{eq}
O2	0.27163 (14)	0.17533 (13)	0.17677 (6)	0.0534 (3)

C15	0.0702 (2)	0.23667 (19)	0.18294 (11)	0.0595 (4)
H15A	−0.0200	0.1425	0.1898	0.089*
H15B	0.0478	0.3119	0.1251	0.089*
H15C	0.0467	0.2971	0.2381	0.089*
O1W	1.07816 (14)	−0.40072 (17)	0.59527 (7)	0.0567 (3)
C9	0.50245 (16)	−0.14171 (14)	0.40181 (8)	0.0360 (3)
N2	0.49491 (14)	−0.31489 (12)	0.55853 (7)	0.0406 (2)
H2	0.3684	−0.2927	0.5657	0.049*
C8	0.60665 (17)	−0.25169 (14)	0.47707 (8)	0.0383 (3)
N1	0.58713 (15)	−0.41549 (12)	0.62992 (7)	0.0412 (3)
C2	0.75138 (18)	−0.64277 (15)	0.77805 (8)	0.0428 (3)
H2A	0.8315	−0.6199	0.7199	0.051*
C12	0.33642 (18)	0.07140 (15)	0.25356 (8)	0.0394 (3)
C1	0.56035 (18)	−0.56972 (15)	0.78779 (8)	0.0401 (3)
C14	0.30309 (17)	−0.08984 (16)	0.41155 (8)	0.0415 (3)
H14	0.2240	−0.1272	0.4683	0.050*
C13	0.21914 (17)	0.01643 (16)	0.33850 (8)	0.0426 (3)
H13	0.0854	0.0506	0.3464	0.051*
C11	0.53540 (19)	0.01912 (17)	0.24265 (9)	0.0471 (3)
H11	0.6139	0.0549	0.1854	0.057*
O1	0.78818 (13)	−0.28143 (12)	0.46533 (7)	0.0538 (3)
F2	0.77810 (17)	−0.89156 (14)	1.01158 (6)	0.0863 (4)
C10	0.61712 (17)	−0.08505 (16)	0.31573 (9)	0.0437 (3)
H10	0.7512	−0.1184	0.3077	0.052*
C7	0.47776 (18)	−0.45989 (15)	0.70817 (8)	0.0420 (3)
H7	0.3451	−0.4224	0.7147	0.050*
F1	1.00444 (13)	−0.82074 (12)	0.84455 (6)	0.0698 (3)
C3	0.82137 (19)	−0.74793 (17)	0.85365 (9)	0.0470 (3)
F3	0.26498 (14)	−0.53644 (14)	0.88906 (7)	0.0779 (3)
C4	0.7048 (2)	−0.78435 (19)	0.93994 (9)	0.0552 (4)
C6	0.4494 (2)	−0.60790 (18)	0.87636 (9)	0.0503 (3)
C5	0.5175 (2)	−0.7150 (2)	0.95292 (9)	0.0613 (4)
H5	0.4386	−0.7390	1.0113	0.074*
H1WA	0.967 (3)	−0.372 (2)	0.5732 (14)	0.079 (5)*
H1WB	1.104 (3)	−0.500 (3)	0.5787 (16)	0.098 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0504 (5)	0.0632 (6)	0.0421 (5)	0.0077 (4)	−0.0084 (4)	0.0111 (4)
C15	0.0544 (8)	0.0629 (9)	0.0585 (8)	0.0126 (6)	−0.0161 (6)	0.0071 (7)
O1W	0.0366 (5)	0.0764 (8)	0.0573 (6)	0.0056 (5)	−0.0114 (4)	−0.0054 (5)
C9	0.0356 (6)	0.0366 (6)	0.0357 (6)	0.0019 (4)	−0.0055 (4)	−0.0028 (5)
N2	0.0345 (5)	0.0445 (5)	0.0405 (5)	0.0045 (4)	−0.0074 (4)	0.0048 (4)
C8	0.0359 (6)	0.0383 (6)	0.0404 (6)	0.0040 (4)	−0.0060 (4)	−0.0029 (5)
N1	0.0417 (5)	0.0398 (5)	0.0412 (5)	0.0021 (4)	−0.0105 (4)	0.0030 (4)
C2	0.0453 (6)	0.0443 (6)	0.0368 (6)	−0.0012 (5)	−0.0033 (5)	0.0016 (5)
C12	0.0425 (6)	0.0401 (6)	0.0351 (6)	0.0006 (5)	−0.0088 (5)	0.0001 (5)

C1	0.0448 (6)	0.0382 (6)	0.0372 (6)	−0.0027 (5)	−0.0077 (5)	−0.0014 (5)
C14	0.0379 (6)	0.0484 (7)	0.0351 (6)	0.0045 (5)	0.0008 (4)	0.0019 (5)
C13	0.0348 (6)	0.0497 (7)	0.0417 (6)	0.0070 (5)	−0.0039 (5)	−0.0006 (5)
C11	0.0410 (6)	0.0597 (8)	0.0368 (6)	−0.0013 (5)	0.0009 (5)	0.0047 (5)
O1	0.0367 (5)	0.0669 (6)	0.0524 (5)	0.0125 (4)	−0.0029 (4)	0.0091 (4)
F2	0.1011 (8)	0.1021 (8)	0.0465 (5)	0.0264 (6)	−0.0128 (5)	0.0238 (5)
C10	0.0324 (6)	0.0540 (7)	0.0423 (6)	0.0037 (5)	−0.0005 (5)	−0.0003 (5)
C7	0.0403 (6)	0.0439 (6)	0.0412 (6)	0.0013 (5)	−0.0076 (5)	−0.0011 (5)
F1	0.0587 (5)	0.0800 (6)	0.0655 (5)	0.0242 (4)	−0.0089 (4)	0.0075 (4)
C3	0.0487 (7)	0.0468 (7)	0.0449 (7)	0.0052 (5)	−0.0089 (5)	−0.0012 (5)
F3	0.0581 (5)	0.1054 (8)	0.0624 (5)	0.0235 (5)	0.0085 (4)	0.0039 (5)
C4	0.0698 (9)	0.0573 (8)	0.0361 (6)	0.0064 (7)	−0.0121 (6)	0.0061 (6)
C6	0.0475 (7)	0.0582 (8)	0.0434 (7)	0.0048 (6)	−0.0013 (5)	−0.0027 (6)
C5	0.0686 (9)	0.0751 (10)	0.0351 (6)	0.0047 (7)	0.0039 (6)	0.0052 (6)

Geometric parameters (Å, º)

O2—C12	1.3606 (13)	C12—C11	1.3860 (17)
O2—C15	1.4210 (16)	C12—C13	1.3863 (16)
C15—H15A	0.9600	C1—C6	1.3846 (17)
C15—H15B	0.9600	C1—C7	1.4605 (15)
C15—H15C	0.9600	C14—C13	1.3861 (15)
O1W—H1WA	0.84 (2)	C14—H14	0.9300
O1W—H1WB	0.86 (2)	C13—H13	0.9300
C9—C14	1.3865 (16)	C11—C10	1.3713 (17)
C9—C10	1.3930 (16)	C11—H11	0.9300
C9—C8	1.4879 (15)	F2—C4	1.3451 (15)
N2—C8	1.3473 (15)	C10—H10	0.9300
N2—N1	1.3747 (13)	C7—H7	0.9300
N2—H2	0.8600	F1—C3	1.3445 (15)
C8—O1	1.2318 (14)	C3—C4	1.3754 (19)
N1—C7	1.2720 (15)	F3—C6	1.3522 (16)
C2—C3	1.3668 (16)	C4—C5	1.363 (2)
C2—C1	1.3936 (17)	C6—C5	1.3794 (18)
C2—H2A	0.9300	C5—H5	0.9300
C12—O2—C15	118.76 (10)	C13—C14—C9	121.42 (10)
O2—C15—H15A	109.5	C13—C14—H14	119.3
O2—C15—H15B	109.5	C9—C14—H14	119.3
H15A—C15—H15B	109.5	C14—C13—C12	119.40 (11)
O2—C15—H15C	109.5	C14—C13—H13	120.3
H15A—C15—H15C	109.5	C12—C13—H13	120.3
H15B—C15—H15C	109.5	C10—C11—C12	120.36 (11)
H1WA—O1W—H1WB	104.7 (19)	C10—C11—H11	119.8
C14—C9—C10	118.11 (10)	C12—C11—H11	119.8
C14—C9—C8	125.20 (10)	C11—C10—C9	121.02 (11)
C10—C9—C8	116.68 (10)	C11—C10—H10	119.5
C8—N2—N1	118.70 (9)	C9—C10—H10	119.5

C8—N2—H2	120.6	N1—C7—C1	120.07 (11)
N1—N2—H2	120.6	N1—C7—H7	120.0
O1—C8—N2	121.75 (10)	C1—C7—H7	120.0
O1—C8—C9	120.98 (10)	F1—C3—C2	120.63 (11)
N2—C8—C9	117.27 (10)	F1—C3—C4	118.54 (11)
C7—N1—N2	115.79 (10)	C2—C3—C4	120.81 (12)
C3—C2—C1	120.19 (11)	F2—C4—C5	120.24 (12)
C3—C2—H2A	119.9	F2—C4—C3	118.74 (13)
C1—C2—H2A	119.9	C5—C4—C3	121.01 (12)
O2—C12—C11	115.34 (10)	F3—C6—C5	118.01 (12)
O2—C12—C13	124.96 (11)	F3—C6—C1	118.64 (12)
C11—C12—C13	119.69 (10)	C5—C6—C1	123.34 (13)
C6—C1—C2	117.04 (11)	C4—C5—C6	117.59 (12)
C6—C1—C7	120.95 (11)	C4—C5—H5	121.2
C2—C1—C7	122.01 (11)	C6—C5—H5	121.2

N1—N2—C8—O1	−0.19 (18)	C14—C9—C10—C11	0.03 (18)
N1—N2—C8—C9	−179.31 (9)	C8—C9—C10—C11	−178.94 (11)
C14—C9—C8—O1	−174.51 (12)	N2—N1—C7—C1	178.74 (9)
C10—C9—C8—O1	4.38 (17)	C6—C1—C7—N1	174.55 (12)
C14—C9—C8—N2	4.62 (18)	C2—C1—C7—N1	−6.50 (18)
C10—C9—C8—N2	−176.49 (11)	C1—C2—C3—F1	179.14 (11)
C8—N2—N1—C7	174.47 (11)	C1—C2—C3—C4	0.5 (2)
C15—O2—C12—C11	−179.01 (12)	F1—C3—C4—F2	−0.2 (2)
C15—O2—C12—C13	1.29 (19)	C2—C3—C4—F2	178.51 (12)
C3—C2—C1—C6	0.47 (18)	F1—C3—C4—C5	−179.57 (13)
C3—C2—C1—C7	−178.52 (11)	C2—C3—C4—C5	−0.9 (2)
C10—C9—C14—C13	−0.51 (18)	C2—C1—C6—F3	178.65 (12)
C8—C9—C14—C13	178.37 (11)	C7—C1—C6—F3	−2.35 (19)
C9—C14—C13—C12	0.39 (19)	C2—C1—C6—C5	−1.1 (2)
O2—C12—C13—C14	179.90 (11)	C7—C1—C6—C5	177.93 (13)
C11—C12—C13—C14	0.21 (19)	F2—C4—C5—C6	−179.08 (14)
O2—C12—C11—C10	179.60 (11)	C3—C4—C5—C6	0.3 (2)
C13—C12—C11—C10	−0.68 (19)	F3—C6—C5—C4	−179.02 (13)
C12—C11—C10—C9	0.6 (2)	C1—C6—C5—C4	0.7 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O1	0.85 (2)	2.05 (2)	2.8376 (13)	154 (2)
O1*W*—H1*WA*···N1	0.85 (2)	2.61 (2)	3.2777 (14)	137 (2)
N2—H2···O1*W*^{i}	0.86	2.12	2.8681 (14)	145
O1*W*—H1*WB*···O1^{ii}	0.86 (2)	2.01 (2)	2.8635 (16)	170 (2)
C5—H5···O2^{iii}	0.93	2.49	3.4128 (15)	172
C7—H7···O1*W*^{i}	0.93	2.54	3.2191 (15)	130

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