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2-Amino-3-((*E*)-{[3-(trifluoromethyl)phenyl]imino}-methyl)-4*H*-chromen-4-one

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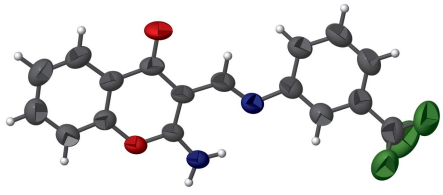
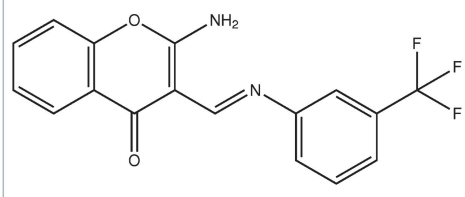
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{17}H_{11}F_3N_2O_2$, the dihedral angle between the chromene ring system and the benzene ring is 19.19 (6)°, and an intramolecular N—H···N hydrogen bond closes an *S*(6) ring. In the crystal, molecules are linked into [100] *C*(6) chains by N—H···O hydrogen bonds.

3D view



Chemical scheme



Structure description

Schiff bases of chromone compounds are known as anticancer agents (Kawase *et al.*, 2007, Barath *et al.*, 2006). As part of our studies in this area, we now describe the synthesis and structure of the title compound, (I).

The dihedral angle between the C2–C7 and C9/C10/O1/C11–C17 ring systems is 19.19 (6)° (Fig. 1); the maximum deviations are 0.012 (2) Å for atom C5 and 0.029 (2) Å for atom C17, respectively. The bond lengths of the imino group atoms [N1—C6 = 1.420 (3) Å and N1—C8 = 1.275 (3) Å] are consistent with corresponding distances in related structures, *i.e.* (*E*)-4-[(4-chlorophenylimino)methyl]benzene-1,2,3-triol (Karabıyık *et al.*, 2008) and (*Z*)-4-({(*Z*)-[2-oxonaphthalen-1(2*H*)-ylidene]methyl}amino)-*N*-[thiazol-2(3*H*)-ylidene]benzenesulfonamide (Köysal *et al.*, 2015). An intramolecular N2—H2*A*···N1 hydrogen bond (Table 1) closes an *R*(6) ring.

In the crystal, N2—H2*B*···O2 hydrogen bonds (Fig. 2) link the molecules into [100] *C*(6) chains.

Synthesis and crystallization

A mixture of a solution containing 2-amino-4-oxo-4*H*-chromene-3-carbaldehyde (0.0076 g 0.040 mmol) in 20 ml ethanol and a solution containing 3-(trifluoromethyl)-aniline (0.0065 g, 0.040 mmol) was refluxed for 1 h in 20 ml ethanol. Crystals of the title

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···N1	0.85 (2)	2.06 (2)	2.727 (2)	134.4 (16)
N2—H2B···O2^{i}	0.90 (2)	1.84 (2)	2.745 (2)	178 (2)

Symmetry code: (i) $x+1, y, z$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{11}F_3N_2O_2$
M_r	332.28
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	293
a, b, c (Å)	7.1355 (7), 7.4786 (8), 14.8254 (18)
α, β, γ (°)	99.626 (9), 91.602 (9), 105.020 (8)
V (Å^3)	751.23 (14)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.12
Crystal size (mm)	0.62 × 0.41 × 0.09
Data collection	
Diffractometer	Stoe IPDS 2
Absorption correction	Integration (*X-RED32*; Stoe & Cie, 2002)
T_{min}, T_{max}	0.928, 0.989
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10651, 3459, 1943
R_{int}	0.035
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.651
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.049, 0.141, 1.00
No. of reflections	3459
No. of parameters	225
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.26, −0.17

Computer programs: *X-AREA* (Stoe & Cie, 2002), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *ORTEP-3 for Windows* (Farrugia, 2012).

compound were obtained from an ethanol solution by slow evaporation (yield 53%; m.p. 471–472 K).

Refinement

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

Acknowledgements

The authors wish to acknowledge the Faculty of Arts and Sciences, Ondokuz Mayıs University,Turkey, for the use of the Stoe IPDS II diffractometer (purchased under grant F.279 of the University Research Fund).

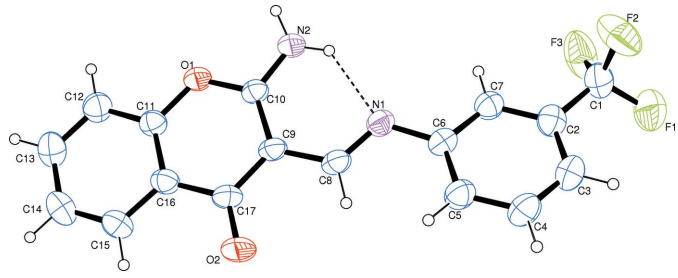


Figure 1
The molecular structure of the title molecule, with displacement ellipsoids drawn at the 30% probability level.

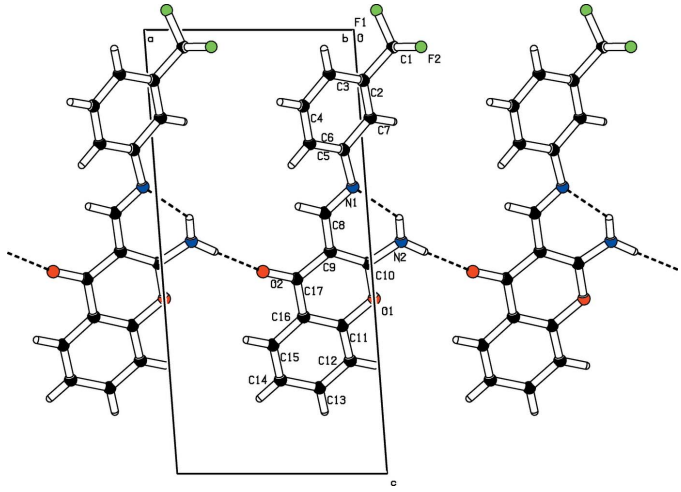


Figure 2
Packing diagram of the title compound, viewed along the *b* axis.

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full crystallographic data

IUCrData (2016). **1**, x160797 [doi:10.1107/S2414314616007975]

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Crystal data

$C_{17}H_{11}F_3N_2O_2$
M_r = 332.28
Triclinic, $P\overline{1}$
a = 7.1355 (7) Å
b = 7.4786 (8) Å
c = 14.8254 (18) Å
α = 99.626 (9)°
β = 91.602 (9)°
γ = 105.020 (8)°
V = 751.23 (14) Å^3
Z = 2
$F(000)$ = 340
D_x = 1.469 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 10185 reflections
θ = 2.8–28.0°
μ = 0.12 mm^{-1}
T = 293 K
Blade, yellow
0.62 × 0.41 × 0.09 mm

Data collection

Stoe IPDS 2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 6.67 pixels mm^{-1}
rotation method scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.928, T_{max} = 0.989
10651 measured reflections
3459 independent reflections
1943 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 27.6°, θ_{min} = 2.8°
h = −9→9
k = −9→9
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.141
S = 1.00
3459 reflections
225 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
$w = 1/[\sigma^2(F_o^2) + (0.0712P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 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.

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
F1	1.1149 (3)	1.2500 (3)	1.04420 (11)	0.1398 (7)
F2	1.3145 (3)	1.3841 (3)	0.96186 (14)	0.1488 (8)
F3	1.2718 (3)	1.0977 (3)	0.96031 (12)	0.1440 (8)
O1	1.00027 (15)	0.60607 (17)	0.39411 (8)	0.0605 (3)
O2	0.48054 (19)	0.7063 (3)	0.45522 (12)	0.1060 (6)
N1	0.9386 (2)	0.9435 (2)	0.64656 (11)	0.0635 (4)
N2	1.1497 (2)	0.7799 (2)	0.52389 (13)	0.0636 (4)
H2A	1.149 (3)	0.848 (3)	0.5759 (15)	0.067 (6)*
H2B	1.257 (3)	0.754 (3)	0.5005 (15)	0.080 (6)*
C1	1.1803 (4)	1.2277 (3)	0.96150 (17)	0.0885 (7)
C2	1.0264 (3)	1.1879 (3)	0.88641 (15)	0.0722 (5)
C3	0.8666 (3)	1.2580 (3)	0.90000 (16)	0.0826 (6)
H3	0.8517	1.3240	0.9571	0.099*
C4	0.7307 (3)	1.2296 (3)	0.82875 (17)	0.0864 (7)
H4	0.6242	1.2790	0.8375	0.104*
C5	0.7485 (3)	1.1285 (3)	0.74360 (15)	0.0750 (6)
H5	0.6554	1.1117	0.6955	0.090*
C6	0.9068 (3)	1.0518 (2)	0.73012 (13)	0.0628 (5)
C7	1.0465 (3)	1.0860 (3)	0.80176 (14)	0.0670 (5)
H7	1.1553	1.0402	0.7932	0.080*
C8	0.7961 (3)	0.8608 (3)	0.58759 (13)	0.0632 (5)
H8	0.6741	0.8746	0.6021	0.076*
C9	0.8082 (2)	0.7480 (2)	0.50068 (13)	0.0578 (4)
C10	0.9849 (2)	0.7136 (2)	0.47434 (12)	0.0542 (4)
C11	0.8380 (2)	0.5221 (2)	0.33411 (13)	0.0590 (4)
C12	0.8643 (3)	0.4088 (3)	0.25495 (15)	0.0741 (5)
H12	0.9866	0.3919	0.2434	0.089*
C13	0.7079 (4)	0.3218 (3)	0.19368 (16)	0.0855 (6)
H13	0.7241	0.2460	0.1396	0.103*
C14	0.5251 (4)	0.3453 (3)	0.21125 (17)	0.0893 (7)
H14	0.4190	0.2840	0.1695	0.107*
C15	0.5009 (3)	0.4590 (3)	0.29012 (16)	0.0807 (6)
H15	0.3781	0.4750	0.3014	0.097*
C16	0.6580 (2)	0.5510 (3)	0.35376 (13)	0.0631 (5)
C17	0.6385 (2)	0.6731 (3)	0.43930 (14)	0.0682 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.1402 (14)	0.1950 (18)	0.0741 (10)	0.0447 (13)	−0.0064 (9)	−0.0010 (10)
F2	0.1259 (13)	0.1278 (13)	0.1574 (17)	−0.0256 (11)	−0.0370 (13)	0.0288 (12)
F3	0.1729 (16)	0.1383 (13)	0.1233 (14)	0.0840 (13)	−0.0604 (12)	−0.0239 (11)
O1	0.0469 (6)	0.0706 (7)	0.0674 (8)	0.0237 (5)	0.0074 (6)	0.0090 (6)
O2	0.0496 (7)	0.1584 (15)	0.1103 (13)	0.0505 (9)	0.0022 (8)	−0.0104 (11)
N1	0.0585 (9)	0.0739 (9)	0.0623 (10)	0.0246 (7)	0.0100 (7)	0.0121 (8)
N2	0.0455 (8)	0.0783 (10)	0.0695 (11)	0.0251 (8)	0.0060 (8)	0.0064 (9)
C1	0.0998 (17)	0.0808 (15)	0.0786 (17)	0.0235 (14)	−0.0026 (13)	−0.0012 (12)
C2	0.0831 (13)	0.0611 (11)	0.0716 (13)	0.0177 (10)	0.0081 (10)	0.0120 (10)
C3	0.1001 (16)	0.0787 (13)	0.0717 (14)	0.0330 (12)	0.0167 (12)	0.0053 (11)
C4	0.0875 (15)	0.0900 (15)	0.0908 (17)	0.0429 (12)	0.0217 (13)	0.0085 (13)
C5	0.0711 (12)	0.0839 (13)	0.0758 (14)	0.0322 (10)	0.0112 (10)	0.0120 (11)
C6	0.0635 (11)	0.0626 (10)	0.0664 (12)	0.0207 (9)	0.0157 (9)	0.0151 (9)
C7	0.0668 (11)	0.0650 (11)	0.0711 (13)	0.0205 (9)	0.0104 (9)	0.0125 (9)
C8	0.0523 (10)	0.0757 (11)	0.0687 (12)	0.0262 (9)	0.0145 (9)	0.0170 (10)
C9	0.0441 (9)	0.0691 (10)	0.0659 (11)	0.0225 (8)	0.0110 (8)	0.0154 (9)
C10	0.0488 (9)	0.0593 (9)	0.0597 (10)	0.0215 (8)	0.0082 (8)	0.0138 (8)
C11	0.0564 (10)	0.0622 (10)	0.0632 (11)	0.0213 (8)	0.0035 (8)	0.0160 (9)
C12	0.0756 (12)	0.0779 (12)	0.0739 (13)	0.0324 (10)	0.0060 (11)	0.0090 (11)
C13	0.1039 (17)	0.0837 (14)	0.0706 (14)	0.0352 (13)	−0.0045 (12)	0.0043 (11)
C14	0.0898 (16)	0.0924 (15)	0.0789 (16)	0.0184 (13)	−0.0228 (13)	0.0113 (13)
C15	0.0606 (11)	0.0990 (15)	0.0825 (15)	0.0232 (11)	−0.0086 (10)	0.0159 (13)
C16	0.0513 (10)	0.0724 (11)	0.0686 (12)	0.0192 (8)	0.0007 (8)	0.0180 (9)
C17	0.0458 (9)	0.0866 (13)	0.0767 (13)	0.0260 (9)	0.0071 (9)	0.0135 (10)

Geometric parameters (Å, º)

F1—C1	1.324 (3)	C5—H5	0.9300
F2—C1	1.304 (3)	C6—C7	1.380 (3)
F3—C1	1.302 (3)	C7—H7	0.9300
O1—C10	1.344 (2)	C8—C9	1.435 (3)
O1—C11	1.380 (2)	C8—H8	0.9300
O2—C17	1.236 (2)	C9—C10	1.404 (2)
N1—C8	1.275 (2)	C9—C17	1.423 (3)
N1—C6	1.420 (2)	C11—C12	1.375 (3)
N2—C10	1.302 (2)	C11—C16	1.388 (2)
N2—H2A	0.85 (2)	C12—C13	1.365 (3)
N2—H2B	0.90 (2)	C12—H12	0.9300
C1—C2	1.479 (3)	C13—C14	1.387 (3)
C2—C3	1.379 (3)	C13—H13	0.9300
C2—C7	1.387 (3)	C14—C15	1.369 (3)
C3—C4	1.365 (3)	C14—H14	0.9300
C3—H3	0.9300	C15—C16	1.395 (3)
C4—C5	1.386 (3)	C15—H15	0.9300
C4—H4	0.9300	C16—C17	1.466 (3)

C5—C6	1.399 (3)

C10—O1—C11	120.17 (13)	N1—C8—H8	117.3
C8—N1—C6	119.83 (15)	C9—C8—H8	117.3
C10—N2—H2A	117.3 (13)	C10—C9—C17	119.43 (17)
C10—N2—H2B	118.3 (13)	C10—C9—C8	121.30 (16)
H2A—N2—H2B	124.4 (19)	C17—C9—C8	119.25 (15)
F3—C1—F2	105.9 (2)	N2—C10—O1	112.79 (14)
F3—C1—F1	105.4 (2)	N2—C10—C9	124.50 (17)
F2—C1—F1	104.0 (2)	O1—C10—C9	122.71 (15)
F3—C1—C2	114.44 (19)	C12—C11—O1	116.69 (16)
F2—C1—C2	112.9 (2)	C12—C11—C16	122.26 (18)
F1—C1—C2	113.3 (2)	O1—C11—C16	121.05 (16)
C3—C2—C7	120.3 (2)	C13—C12—C11	118.85 (19)
C3—C2—C1	119.7 (2)	C13—C12—H12	120.6
C7—C2—C1	119.89 (19)	C11—C12—H12	120.6
C4—C3—C2	119.3 (2)	C12—C13—C14	120.7 (2)
C4—C3—H3	120.3	C12—C13—H13	119.7
C2—C3—H3	120.3	C14—C13—H13	119.7
C3—C4—C5	121.1 (2)	C15—C14—C13	119.9 (2)
C3—C4—H4	119.4	C15—C14—H14	120.0
C5—C4—H4	119.4	C13—C14—H14	120.0
C4—C5—C6	119.8 (2)	C14—C15—C16	120.8 (2)
C4—C5—H5	120.1	C14—C15—H15	119.6
C6—C5—H5	120.1	C16—C15—H15	119.6
C7—C6—C5	118.56 (18)	C11—C16—C15	117.49 (19)
C7—C6—N1	116.63 (16)	C11—C16—C17	119.89 (16)
C5—C6—N1	124.79 (18)	C15—C16—C17	122.62 (17)
C6—C7—C2	120.72 (18)	O2—C17—C9	123.26 (19)
C6—C7—H7	119.6	O2—C17—C16	120.15 (18)
C2—C7—H7	119.6	C9—C17—C16	116.60 (15)
N1—C8—C9	125.45 (16)		

F3—C1—C2—C3	150.4 (2)	C8—C9—C10—N2	−0.8 (3)
F2—C1—C2—C3	−88.4 (3)	C17—C9—C10—O1	−2.5 (3)
F1—C1—C2—C3	29.6 (3)	C8—C9—C10—O1	178.87 (16)
F3—C1—C2—C7	−31.8 (3)	C10—O1—C11—C12	−177.75 (16)
F2—C1—C2—C7	89.4 (3)	C10—O1—C11—C16	2.0 (2)
F1—C1—C2—C7	−152.7 (2)	O1—C11—C12—C13	179.66 (19)
C7—C2—C3—C4	−1.4 (3)	C16—C11—C12—C13	−0.1 (3)
C1—C2—C3—C4	176.3 (2)	C11—C12—C13—C14	−0.7 (3)
C2—C3—C4—C5	1.3 (4)	C12—C13—C14—C15	1.0 (4)
C3—C4—C5—C6	0.8 (3)	C13—C14—C15—C16	−0.4 (4)
C4—C5—C6—C7	−2.7 (3)	C12—C11—C16—C15	0.6 (3)
C4—C5—C6—N1	178.99 (19)	O1—C11—C16—C15	−179.16 (18)
C8—N1—C6—C7	159.66 (18)	C12—C11—C16—C17	179.95 (18)
C8—N1—C6—C5	−22.0 (3)	O1—C11—C16—C17	0.2 (3)
C5—C6—C7—C2	2.5 (3)	C14—C15—C16—C11	−0.3 (3)

N1—C6—C7—C2	−179.00 (17)	C14—C15—C16—C17	−179.7 (2)
C3—C2—C7—C6	−0.5 (3)	C10—C9—C17—O2	−175.6 (2)
C1—C2—C7—C6	−178.25 (19)	C8—C9—C17—O2	3.0 (3)
C6—N1—C8—C9	179.79 (18)	C10—C9—C17—C16	4.4 (3)
N1—C8—C9—C10	2.3 (3)	C8—C9—C17—C16	−176.88 (17)
N1—C8—C9—C17	−176.31 (19)	C11—C16—C17—O2	176.7 (2)
C11—O1—C10—N2	178.83 (15)	C15—C16—C17—O2	−4.0 (3)
C11—O1—C10—C9	−0.9 (2)	C11—C16—C17—C9	−3.4 (3)
C17—C9—C10—N2	177.86 (18)	C15—C16—C17—C9	175.96 (19)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···N1	0.85 (2)	2.06 (2)	2.727 (2)	134.4 (16)
N2—H2*B*···O2^{i}	0.90 (2)	1.84 (2)	2.745 (2)	178 (2)

Symmetry code: (i) *x*+1, *y*, *z*.