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(*E*)-4-Bromo-*N*′-[(5-methylfuran-2-yl)-methylene]benzohydrazide

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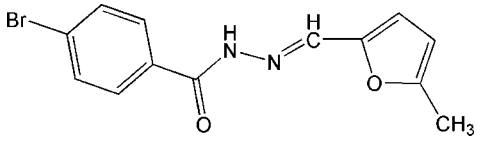
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.005 Å; R factor = 0.041; wR factor = 0.104; data-to-parameter ratio = 13.3.

The asymmetric unit of the title compound, $C_{13}H_{11}BrN_2O_2$, contains two independent molecules. In one molecule, the dihedral angle between the two ring planes is 28.10 (3)°; in the other, it is 28.90 (3)°. Intermolecular N—H···O hydrogen bonds link the molecules to form a three-dimensional network.

Related literature

For general background, see: Belloni *et al.* (2005); Kahwa *et al.* (1986); Parashar *et al.* (1988); Santos *et al.* (2001); Tynan *et al.* (2005).



Experimental

Crystal data

$C_{13}H_{11}BrN_2O_2$
M_r = 307.15
Triclinic, $P\overline{1}$
a = 8.0276 (13) Å
b = 10.0734 (16) Å
c = 16.458 (3) Å
α = 105.166 (3)°
β = 94.668 (3)°
γ = 90.576 (3)°
V = 1279.6 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.21 mm^{-1}
T = 294 (2) K
0.20 × 0.18 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.566, T_{max} = 0.628
6684 measured reflections
4482 independent reflections
3125 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.104
S = 1.02
4482 reflections
336 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4A···O2^{i}	0.889 (10)	2.089 (14)	2.929 (3)	157 (2)
N2—H2A···O4	0.890 (10)	2.088 (14)	2.950 (3)	163 (3)

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

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2374).

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supplementary materials

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(*E*)-4-Bromo-*N*'-[(5-methylfuran-2-yl)methylene]benzohydrazide

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Comment

In order to establish control over the preparation of crystalline solid materials so that their architecture and properties are predictable (Belloni *et al.*, 2005; Tynan *et al.*, 2005; Parashar *et al.*, 1988), the synthesis of new and designed crystal structures has become a major strand of modern chemistry. Metal complexes based on Schiff bases have attracted much attention because they can be utilized as model compounds of the active centres in various proteins and enzymes (Kahwa *et al.*, 1986; Santos *et al.*,2001). As part of an investigation of the coordination properties of Shiff bases functioning as ligands, we report the synthesis and crystal structure of the title compound, (I).

In the structure of the title molecule (I) (Fig. 1), the geometric parameters are normal. In the one molecule of the unit, the furan ring (C2—C5/O1) is approximately planar, with a maximum deviation from the mean plane of 0.0023 (2) Å for atom O1, as are the benzene group (C8—C13) is approximately planar, with a maximum deviation from the mean plane of 0.0060 (5) Å. The dihedral angle between these two planes is 28.10 (3)°. In the other molecule of the unit, the furan ring (C15—C18/O3) is approximately planar, with a maximum deviation from the mean plane of 0.0019 (2) Å for atom O3, as are the benzene group (C21—C26) is approximately planar, with a maximum deviation from the mean plane of 0.0069 (4) Å. The dihedral angle between these two planes is 28.90 (3)°. Intermolecular N—H···O hydrogen bonds link the molecules to form a three-dimensional network, as illustraed in Fig.2 and Table 1.

Experimental

An anhydrous ethanol solution (50 ml) of 4-bromobenzohydrazide (2.14 g, 10 mmol) was added to an anhydrous ethanol solution (50 ml) of 5-methylfuran-2-carbaldehyde (1.10 g, 10 mmol), and the mixture was stirred at 350 K for 6 h under N_2, whereupon a red precipitate appeared. The product was isolated, recrystallized from anhydrous ethanol and then dried *in vacuo* to give pure compound (I) in 91% yield. Red single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an anhydrous ethanol solution.

Refinement

The N-bound H atom was located in a difference Fourier map and refined freely. C-bound H atoms were included in calculated positions, with C—H = 0.93 (aromatic) or 0.96 Å (methyl), and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic H or $1.5U_{eq}(C)$ for methyl H atoms.

Figures

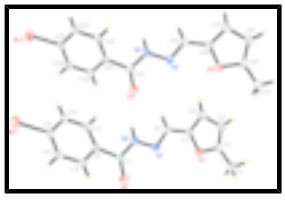

Fig. 1. The structure of the title molecule (I). Displacement ellipsoids are drawn at the 30% probability level.

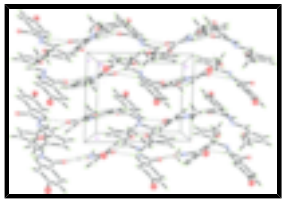

Fig. 2. The crystal packing of (I). Hydrogen bonds are indicated by dashed lines.

(*E*)-4-Bromo-*N*'-[(5-methylfuran-2-yl)methylene]benzohydrazide

Crystal data

$C_{13}H_{11}BrN_2O_2$	$Z = 4$
$M_r = 307.15$	$F_{000} = 616$
Triclinic, $P\overline{1}$	$D_x = 1.594$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.0276$ (13) Å	Cell parameters from 2664 reflections
$b = 10.0734$ (16) Å	$\theta = 3.3$–26.4°
$c = 16.458$ (3) Å	$\mu = 3.21$ mm^{-1}
$\alpha = 105.166$ (3)°	$T = 294$ (2) K
$\beta = 94.668$ (3)°	Block, red
$\gamma = 90.576$ (3)°	0.20 × 0.18 × 0.16 mm
$V = 1279.6$ (4) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	4482 independent reflections
Radiation source: fine-focus sealed tube	3125 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.036$
$T = 294$(2) K	$\theta_{max} = 25.0^\circ$
φ and ω scans	$\theta_{min} = 2.1^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -9 \rightarrow 8$
$T_{min} = 0.566$, $T_{max} = 0.628$	$k = -11 \rightarrow 11$
6684 measured reflections	$l = -18 \rightarrow 19$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.041$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.104$	$w = 1/[\sigma^2(F_o^2) + (0.0417P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.001$
4482 reflections	$\Delta\rho_{max} = 0.50$ e Å^{-3}
336 parameters	$\Delta\rho_{min} = -0.64$ e Å^{-3}
2 restraints	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0259 (15)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) 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. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.44683 (6)	0.33727 (4)	0.10793 (2)	0.06531 (18)
Br2	0.82935 (6)	0.82934 (4)	0.09703 (2)	0.06943 (19)
O1	0.9618 (3)	0.5777 (2)	0.77720 (14)	0.0454 (6)
O2	0.6940 (4)	0.2664 (2)	0.49922 (14)	0.0668 (8)
O3	0.6924 (3)	1.0721 (2)	0.78316 (13)	0.0468 (6)
O4	0.8046 (4)	0.7674 (2)	0.49693 (14)	0.0661 (8)
N1	0.8312 (4)	0.5044 (3)	0.60515 (17)	0.0454 (7)
N2	0.7656 (4)	0.4902 (3)	0.52273 (17)	0.0455 (7)
N3	0.7319 (4)	1.0057 (3)	0.60812 (16)	0.0450 (7)
N4	0.7522 (4)	0.9927 (3)	0.52433 (17)	0.0456 (7)
C1	1.0508 (6)	0.5719 (4)	0.9199 (2)	0.0724 (12)
H1A	1.0758	0.6347	0.9746	0.109*
H1B	1.1425	0.5118	0.9066	0.109*
H1C	0.9513	0.5183	0.9201	0.109*
C2	1.0243 (5)	0.6503 (4)	0.8557 (2)	0.0492 (9)
C3	1.0466 (5)	0.7819 (4)	0.8572 (3)	0.0625 (11)
H3	1.0876	0.8524	0.9036	0.075*
C4	0.9965 (5)	0.7946 (4)	0.7760 (3)	0.0588 (10)
H4	0.9976	0.8749	0.7582	0.071*

C5	0.9472 (4)	0.6694 (3)	0.7295 (2)	0.0447 (8)
C6	0.8793 (4)	0.6266 (3)	0.6434 (2)	0.0457 (9)
H6	0.8697	0.6930	0.6134	0.055*
C7	0.7004 (4)	0.3704 (3)	0.4743 (2)	0.0431 (8)
C8	0.6356 (4)	0.3699 (3)	0.3872 (2)	0.0381 (8)
C9	0.5169 (4)	0.2708 (3)	0.3442 (2)	0.0464 (9)
H9	0.4754	0.2092	0.3715	0.056*
C10	0.4596 (4)	0.2615 (3)	0.2627 (2)	0.0464 (9)
H10	0.3791	0.1945	0.2346	0.056*
C11	0.5224 (4)	0.3526 (3)	0.2223 (2)	0.0423 (8)
C12	0.6365 (4)	0.4532 (3)	0.2634 (2)	0.0462 (9)
H12	0.6751	0.5158	0.2359	0.055*
C13	0.6945 (4)	0.4622 (3)	0.3451 (2)	0.0468 (9)
H13	0.7738	0.5304	0.3729	0.056*
C14	0.6697 (6)	1.0567 (4)	0.9257 (2)	0.0773 (13)
H14A	0.6649	1.1158	0.9815	0.116*
H14B	0.7712	1.0067	0.9232	0.116*
H14C	0.5754	0.9930	0.9122	0.116*
C15	0.6659 (5)	1.1406 (4)	0.8640 (2)	0.0516 (9)
C16	0.6427 (5)	1.2732 (4)	0.8694 (2)	0.0571 (10)
H16	0.6233	1.3411	0.9178	0.068*
C17	0.6530 (5)	1.2912 (3)	0.7882 (2)	0.0537 (10)
H17	0.6410	1.3731	0.7726	0.064*
C18	0.6834 (4)	1.1680 (3)	0.7377 (2)	0.0427 (8)
C19	0.7053 (4)	1.1292 (3)	0.6498 (2)	0.0450 (8)
H19	0.7001	1.1972	0.6209	0.054*
C20	0.7872 (4)	0.8710 (3)	0.4727 (2)	0.0430 (8)
C21	0.8010 (4)	0.8691 (3)	0.3830 (2)	0.0372 (8)
C22	0.8982 (4)	0.7703 (3)	0.3355 (2)	0.0437 (8)
H22	0.9568	0.7107	0.3611	0.052*
C23	0.9093 (4)	0.7592 (3)	0.2514 (2)	0.0454 (9)
H23	0.9757	0.6932	0.2199	0.054*
C24	0.8203 (4)	0.8474 (3)	0.2142 (2)	0.0424 (8)
C25	0.7257 (4)	0.9477 (3)	0.2597 (2)	0.0487 (9)
H25	0.6682	1.0076	0.2339	0.058*
C26	0.7172 (4)	0.9581 (3)	0.3436 (2)	0.0452 (9)
H26	0.6539	1.0265	0.3751	0.054*
H4A	0.755 (3)	1.0683 (18)	0.5062 (16)	0.029 (8)*
H2A	0.767 (4)	0.566 (2)	0.5041 (19)	0.050 (10)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0881 (3)	0.0599 (3)	0.0407 (3)	0.0095 (2)	−0.0034 (2)	0.00281 (18)
Br2	0.1012 (4)	0.0675 (3)	0.0386 (3)	0.0067 (2)	0.0212 (2)	0.00751 (19)
O1	0.0665 (16)	0.0364 (13)	0.0347 (13)	0.0082 (11)	0.0074 (12)	0.0106 (11)
O2	0.122 (3)	0.0350 (14)	0.0487 (17)	0.0049 (14)	0.0062 (15)	0.0197 (12)
O3	0.0699 (16)	0.0367 (13)	0.0333 (13)	0.0042 (11)	0.0134 (11)	0.0058 (10)

O4	0.120 (2)	0.0339 (14)	0.0502 (17)	0.0105 (14)	0.0149 (15)	0.0183 (12)
N1	0.063 (2)	0.0404 (17)	0.0360 (17)	0.0135 (14)	0.0060 (14)	0.0143 (13)
N2	0.071 (2)	0.0333 (16)	0.0354 (17)	0.0097 (14)	0.0035 (15)	0.0154 (13)
N3	0.065 (2)	0.0402 (17)	0.0318 (16)	−0.0005 (14)	0.0102 (14)	0.0123 (13)
N4	0.078 (2)	0.0289 (15)	0.0347 (17)	0.0030 (14)	0.0160 (15)	0.0135 (13)
C1	0.117 (4)	0.067 (3)	0.034 (2)	0.008 (2)	0.002 (2)	0.016 (2)
C2	0.064 (2)	0.046 (2)	0.035 (2)	0.0087 (17)	0.0072 (18)	0.0044 (16)
C3	0.077 (3)	0.046 (2)	0.055 (3)	0.0001 (19)	−0.009 (2)	0.0002 (19)
C4	0.073 (3)	0.039 (2)	0.064 (3)	−0.0021 (18)	−0.003 (2)	0.0158 (19)
C5	0.051 (2)	0.039 (2)	0.047 (2)	0.0103 (16)	0.0066 (17)	0.0159 (17)
C6	0.055 (2)	0.039 (2)	0.047 (2)	0.0092 (16)	0.0057 (18)	0.0181 (17)
C7	0.061 (2)	0.0298 (18)	0.041 (2)	0.0099 (16)	0.0175 (17)	0.0102 (16)
C8	0.050 (2)	0.0268 (17)	0.0392 (19)	0.0098 (15)	0.0139 (16)	0.0088 (15)
C9	0.058 (2)	0.0315 (18)	0.054 (2)	0.0066 (16)	0.0196 (19)	0.0145 (17)
C10	0.052 (2)	0.0310 (18)	0.052 (2)	0.0043 (15)	0.0082 (18)	0.0035 (17)
C11	0.050 (2)	0.0394 (19)	0.0337 (19)	0.0127 (16)	0.0098 (16)	0.0014 (15)
C12	0.062 (2)	0.042 (2)	0.038 (2)	−0.0022 (17)	0.0073 (18)	0.0149 (16)
C13	0.054 (2)	0.044 (2)	0.041 (2)	−0.0036 (16)	0.0040 (17)	0.0090 (17)
C14	0.131 (4)	0.065 (3)	0.037 (2)	0.010 (3)	0.017 (2)	0.011 (2)
C15	0.074 (3)	0.046 (2)	0.032 (2)	0.0007 (18)	0.0108 (18)	0.0027 (16)
C16	0.075 (3)	0.045 (2)	0.045 (2)	0.0040 (19)	0.015 (2)	−0.0027 (18)
C17	0.072 (3)	0.037 (2)	0.054 (2)	0.0098 (17)	0.015 (2)	0.0099 (17)
C18	0.054 (2)	0.0362 (19)	0.041 (2)	0.0020 (15)	0.0132 (17)	0.0140 (16)
C19	0.062 (2)	0.037 (2)	0.040 (2)	0.0011 (16)	0.0106 (17)	0.0139 (16)
C20	0.057 (2)	0.0327 (19)	0.042 (2)	0.0011 (15)	0.0071 (17)	0.0142 (16)
C21	0.048 (2)	0.0266 (16)	0.0378 (19)	0.0003 (14)	0.0104 (16)	0.0084 (14)
C22	0.053 (2)	0.0297 (17)	0.050 (2)	0.0050 (15)	0.0070 (17)	0.0119 (15)
C23	0.052 (2)	0.0341 (18)	0.047 (2)	0.0051 (15)	0.0142 (17)	0.0022 (16)
C24	0.053 (2)	0.0409 (19)	0.0308 (18)	−0.0043 (16)	0.0123 (16)	0.0019 (15)
C25	0.063 (2)	0.044 (2)	0.041 (2)	0.0154 (17)	0.0097 (18)	0.0128 (16)
C26	0.058 (2)	0.0387 (19)	0.039 (2)	0.0147 (16)	0.0120 (17)	0.0088 (16)

Geometric parameters (Å, °)

Br1—C11	1.897 (3)	C9—C10	1.361 (5)
Br2—C24	1.896 (3)	C9—H9	0.9300
O1—C2	1.359 (4)	C10—C11	1.380 (5)
O1—C5	1.360 (4)	C10—H10	0.9300
O2—C7	1.222 (3)	C11—C12	1.358 (5)
O3—C15	1.363 (4)	C12—C13	1.367 (5)
O3—C18	1.367 (4)	C12—H12	0.9300
O4—C20	1.217 (3)	C13—H13	0.9300
N1—C6	1.268 (4)	C14—C15	1.480 (5)
N1—N2	1.385 (4)	C14—H14A	0.9600
N2—C7	1.335 (4)	C14—H14B	0.9600
N2—H2A	0.890 (10)	C14—H14C	0.9600
N3—C19	1.283 (4)	C15—C16	1.331 (5)
N3—N4	1.374 (3)	C16—C17	1.403 (5)
N4—C20	1.343 (4)	C16—H16	0.9300

N4—H4A	0.889 (10)	C17—C18	1.339 (4)
C1—C2	1.479 (5)	C17—H17	0.9300
C1—H1A	0.9600	C18—C19	1.423 (4)
C1—H1B	0.9600	C19—H19	0.9300
C1—H1C	0.9600	C20—C21	1.483 (4)
C2—C3	1.329 (5)	C21—C22	1.385 (4)
C3—C4	1.403 (5)	C21—C26	1.386 (4)
C3—H3	0.9300	C22—C23	1.370 (5)
C4—C5	1.330 (5)	C22—H22	0.9300
C4—H4	0.9300	C23—C24	1.379 (5)
C5—C6	1.429 (5)	C23—H23	0.9300
C6—H6	0.9300	C24—C25	1.368 (5)
C7—C8	1.484 (5)	C25—C26	1.366 (4)
C8—C9	1.381 (5)	C25—H25	0.9300
C8—C13	1.396 (4)	C26—H26	0.9300
C2—O1—C5	106.3 (3)	C11—C12—H12	120.1
C15—O3—C18	106.1 (2)	C13—C12—H12	120.1
C6—N1—N2	113.3 (3)	C12—C13—C8	120.5 (3)
C7—N2—N1	121.7 (3)	C12—C13—H13	119.8
C7—N2—H2A	122 (2)	C8—C13—H13	119.8
N1—N2—H2A	116 (2)	C15—C14—H14A	109.5
C19—N3—N4	113.6 (3)	C15—C14—H14B	109.5
C20—N4—N3	121.1 (3)	H14A—C14—H14B	109.5
C20—N4—H4A	119.8 (18)	C15—C14—H14C	109.5
N3—N4—H4A	118.7 (18)	H14A—C14—H14C	109.5
C2—C1—H1A	109.5	H14B—C14—H14C	109.5
C2—C1—H1B	109.5	C16—C15—O3	110.1 (3)
H1A—C1—H1B	109.5	C16—C15—C14	133.9 (3)
C2—C1—H1C	109.5	O3—C15—C14	115.9 (3)
H1A—C1—H1C	109.5	C15—C16—C17	107.1 (3)
H1B—C1—H1C	109.5	C15—C16—H16	126.4
C3—C2—O1	109.8 (3)	C17—C16—H16	126.4
C3—C2—C1	133.7 (4)	C18—C17—C16	106.8 (3)
O1—C2—C1	116.5 (3)	C18—C17—H17	126.6
C2—C3—C4	107.2 (3)	C16—C17—H17	126.6
C2—C3—H3	126.4	C17—C18—O3	109.8 (3)
C4—C3—H3	126.4	C17—C18—C19	129.9 (3)
C5—C4—C3	106.5 (3)	O3—C18—C19	120.3 (3)
C5—C4—H4	126.7	N3—C19—C18	123.7 (3)
C3—C4—H4	126.7	N3—C19—H19	118.2
C4—C5—O1	110.2 (3)	C18—C19—H19	118.2
C4—C5—C6	129.2 (3)	O4—C20—N4	122.6 (3)
O1—C5—C6	120.6 (3)	O4—C20—C21	121.4 (3)
N1—C6—C5	124.4 (3)	N4—C20—C21	116.0 (3)
N1—C6—H6	117.8	C22—C21—C26	118.3 (3)
C5—C6—H6	117.8	C22—C21—C20	118.3 (3)
O2—C7—N2	122.8 (3)	C26—C21—C20	123.4 (3)
O2—C7—C8	121.3 (3)	C23—C22—C21	121.0 (3)
N2—C7—C8	115.9 (3)	C23—C22—H22	119.5

C9—C8—C13	118.2 (3)	C21—C22—H22	119.5
C9—C8—C7	119.0 (3)	C22—C23—C24	118.8 (3)
C13—C8—C7	122.8 (3)	C22—C23—H23	120.6
C10—C9—C8	121.3 (3)	C24—C23—H23	120.6
C10—C9—H9	119.3	C25—C24—C23	121.7 (3)
C8—C9—H9	119.3	C25—C24—Br2	119.1 (3)
C9—C10—C11	119.1 (3)	C23—C24—Br2	119.2 (2)
C9—C10—H10	120.4	C26—C25—C24	118.7 (3)
C11—C10—H10	120.4	C26—C25—H25	120.6
C12—C11—C10	121.0 (3)	C24—C25—H25	120.6
C12—C11—Br1	119.7 (3)	C25—C26—C21	121.5 (3)
C10—C11—Br1	119.3 (3)	C25—C26—H26	119.2
C11—C12—C13	119.8 (3)	C21—C26—H26	119.2
C6—N1—N2—C7	−176.3 (3)	C7—C8—C13—C12	176.8 (3)
C19—N3—N4—C20	177.5 (3)	C18—O3—C15—C16	−0.4 (4)
C5—O1—C2—C3	0.5 (4)	C18—O3—C15—C14	179.9 (3)
C5—O1—C2—C1	179.7 (3)	O3—C15—C16—C17	0.6 (4)
O1—C2—C3—C4	−0.2 (5)	C14—C15—C16—C17	−179.9 (5)
C1—C2—C3—C4	−179.2 (4)	C15—C16—C17—C18	−0.5 (5)
C2—C3—C4—C5	−0.3 (5)	C16—C17—C18—O3	0.2 (4)
C3—C4—C5—O1	0.6 (4)	C16—C17—C18—C19	−179.8 (4)
C3—C4—C5—C6	177.6 (4)	C15—O3—C18—C17	0.1 (4)
C2—O1—C5—C4	−0.7 (4)	C15—O3—C18—C19	−179.8 (3)
C2—O1—C5—C6	−178.0 (3)	N4—N3—C19—C18	−178.9 (3)
N2—N1—C6—C5	178.2 (3)	C17—C18—C19—N3	−179.0 (4)
C4—C5—C6—N1	−177.9 (4)	O3—C18—C19—N3	0.9 (5)
O1—C5—C6—N1	−1.2 (5)	N3—N4—C20—O4	−0.9 (5)
N1—N2—C7—O2	0.2 (5)	N3—N4—C20—C21	178.2 (3)
N1—N2—C7—C8	−179.6 (3)	O4—C20—C21—C22	−26.4 (5)
O2—C7—C8—C9	23.0 (5)	N4—C20—C21—C22	154.5 (3)
N2—C7—C8—C9	−157.2 (3)	O4—C20—C21—C26	151.4 (3)
O2—C7—C8—C13	−154.3 (3)	N4—C20—C21—C26	−27.7 (5)
N2—C7—C8—C13	25.5 (5)	C26—C21—C22—C23	−1.1 (5)
C13—C8—C9—C10	0.8 (5)	C20—C21—C22—C23	176.8 (3)
C7—C8—C9—C10	−176.7 (3)	C21—C22—C23—C24	−0.6 (5)
C8—C9—C10—C11	0.4 (5)	C22—C23—C24—C25	1.9 (5)
C9—C10—C11—C12	−1.8 (5)	C22—C23—C24—Br2	−178.1 (2)
C9—C10—C11—Br1	178.5 (2)	C23—C24—C25—C26	−1.3 (5)
C10—C11—C12—C13	2.0 (5)	Br2—C24—C25—C26	178.7 (3)
Br1—C11—C12—C13	−178.2 (3)	C24—C25—C26—C21	−0.5 (5)
C11—C12—C13—C8	−0.9 (5)	C22—C21—C26—C25	1.7 (5)
C9—C8—C13—C12	−0.5 (5)	C20—C21—C26—C25	−176.1 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4A···O2^{i}	0.889 (10)	2.089 (14)	2.929 (3)	157 (2)
N2—H2A···O4	0.890 (10)	2.088 (14)	2.950 (3)	163 (3)

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

Fig. 1

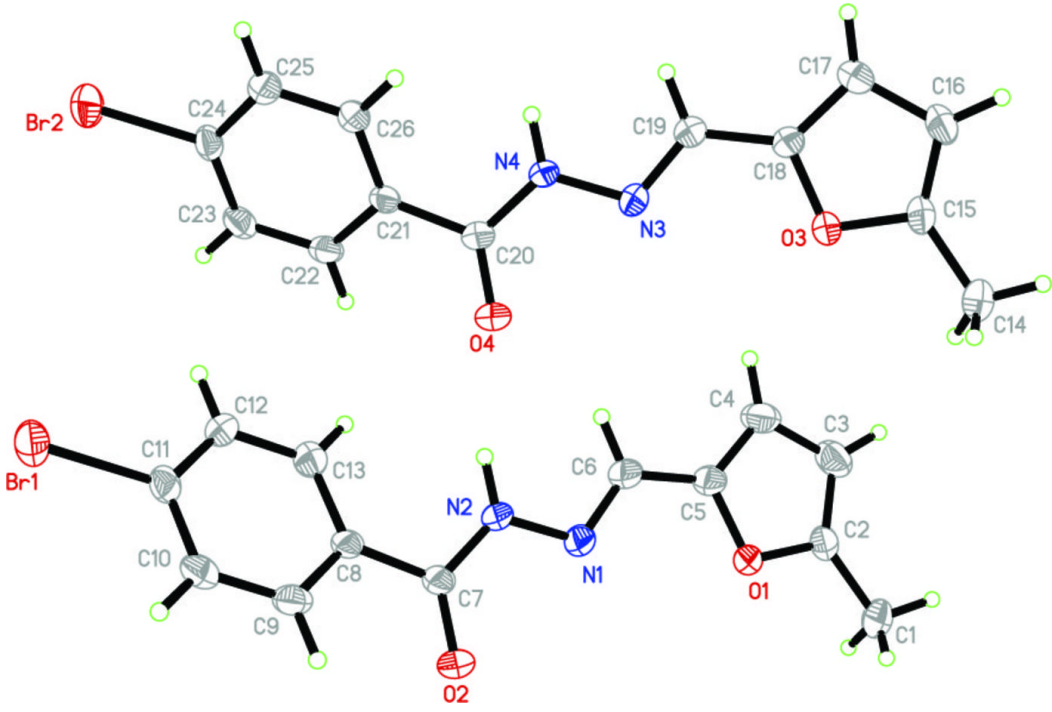
Br2
C25
C24
C26
C23
C21
C22
C20
O4
N4
N3
C19
C17
C16
C18
C15
O3
C14
Br1
C12
C11
C13
C10
C8
C9
C7
O2
N2
N1
C6
C4
C3
C5
C2
O1
C1

Fig. 2