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4-Methoxy-*N*-[(1*E*)-(2-nitrophenyl)-methylene]benzhydrazide

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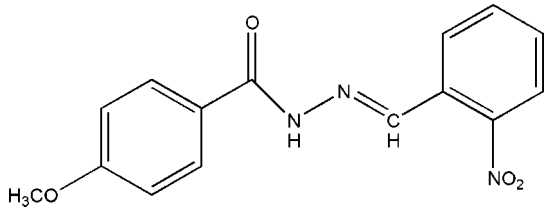
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.005 Å; R factor = 0.037; wR factor = 0.094; data-to-parameter ratio = 6.5.

The structure of the title molecule, $C_{15}H_{13}N_3O_4$, is stabilized by intermolecular N—H···O hydrogen bonds. There are two crystallographically independent molecules in the asymmetric unit. The dihedral angles between the benzene rings in the two molecules are 86.75 (9) and 8.3 (2)°.

Related literature

For related literature, see: Carcelli *et al.* (1995); Salem (1998); Singh *et al.* (1982).



Experimental

Crystal data

$C_{15}H_{13}N_3O_4$
M_r = 299.28
Orthorhombic, $Pca2_1$
a = 27.3272 (15) Å
b = 4.8389 (3) Å
c = 21.6639 (12) Å
V = 2864.7 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 273 (2) K
0.35 × 0.23 × 0.13 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.966, T_{max} = 0.983
24492 measured reflections
2598 independent reflections
2106 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.094
S = 1.08
2598 reflections
400 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.11 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.86	1.99	2.769 (3)	150
N4—H4···O5^{i}	0.86	2.01	2.819 (3)	156

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FI2043).

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supplementary materials

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4-Methoxy-*N*-[(1*E*)-(2-nitrophenyl)methylene]benzhydrazide

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Comment

The chemistry of aroylhydrazones continues to attract much attention due to their coordination ability to metal ions (Singh *et al.*, 1982; Salem, 1998) and their biological activity (Singh *et al.*, 1982; Carcelli *et al.*, 1995). As an extension of the work on the structural characterization of aroylhydrazone derivatives, the title compound, (I),was synthesized and its crystal structure is reported here.

There are two crystallographically independent molecules in the asymmetric unit (Fig. 1). The conformations of the two molecules are almost the same. Both display *trans* conformation with respect to the C9=N2 and C24=N5 double bond. The benzene rings of the two molecules, C2—C7(A), C10—C15(B), C17—C22(C) and C25—C30(D), make dihedral angles of 86.75 (9)° (A;B), but 8.3 (2)°(C;D)·The crystal structure is stabilized by intermolecular N—H···O hydrogen bonds, which yield chains running along *b*. (Table 1. and Fig. 2).

Experimental

4-methoxybenzohydrazide (0.01 mol,1.66 g) was dissolved in anhydrous ethanol (50 ml), and 2-nitrobenzaldehyde (Shanghai Chemical Reagents Company, 99%, 0.01 mol, 1.51 g) was added. The reaction mixture was refluxed for 4 h with stirring, then the resulting precipitate was collected by filtration, washed several times with ethanol and dried *in vacuo* (yield 85%). The compound (1.0 mmol,0.30 g) was dissolved in dimethylformamide (15 ml) and kept at room temperature for 30 d to obtain yellow single crystals suitable for X-ray diffraction.

Refinement

Friedel pairs were merged prior to refinement. All H atoms were positioned geometrically and treated as riding on their parent atoms,with *C*—*H*(methyl) = 0.96 Å, *C*—*H*(aromatic,imine) = 0.93 Å, and N—H = 0.86 Å and with U_{iso}(H) =1.5U_{eq}($C_{methyl,}$) and 1.2U_{eq}($C_{aromatic}$,C_{imine},*N*).

Figures

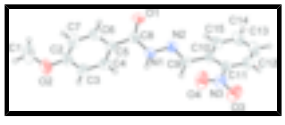

Fig. 1. The molecular structures of one of the two molecules of compound (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

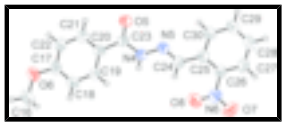

Fig. 2. The molecular structures of other of the two molecules of compound (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

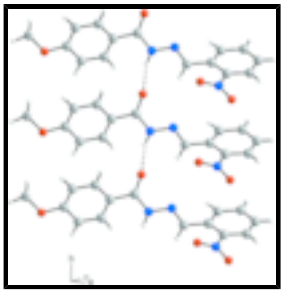

Fig. 3. The chains in (I), formed by hydrogen bonding. Dashed lines show intermolecular hydrogen bonds.

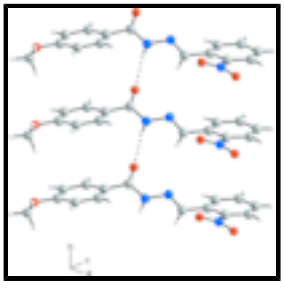

Fig. 4. The chains in (I), formed by hydrogen bonding. Dashed lines show intermolecular hydrogen bonds.

4-methoxy-*N*-[(1E)-(2-nitrophenyl)methylene]benzhydrazide

Crystal data

$C_{15}H_{13}N_3O_4$	F_{000} = 1248
M_r = 299.28	D_x = 1.388 Mg m^{-3}
Orthorhombic, *Pca*2$_1$	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: P 2c -2ac	Cell parameters from 3567 reflections
a = 27.3272 (15) Å	θ = 2.4–21.4º
b = 4.8389 (3) Å	μ = 0.10 mm^{-1}
c = 21.6639 (12) Å	*T* = 273 (2) K
V = 2864.7 (3) Å^3	Block, yellow
Z = 8	0.35 × 0.23 × 0.13 mm

Data collection

Bruker APEX II CCD diffractometer	2598 independent reflections
Radiation source: fine-focus sealed tube	2106 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.055
T = 273(2) K	θ_{max} = 25.0º
φ & ω scans	θ_{min} = 1.5º
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	*h* = −32→32
T_{min} = 0.966, T_{max} = 0.983	*k* = −5→5
24492 measured reflections	*l* = −25→25

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.037$

$wR(F^2) = 0.094$

$S = 1.08$

2598 reflections

400 parameters

1 restraint

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.055P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = <0.001$

$\Delta\rho_{max} = 0.15$ e Å^{-3}

$\Delta\rho_{min} = -0.11$ e Å^{-3}

Extinction correction: SHELXL97,
$Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0052 (8)

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}
O1	0.95758 (9)	0.5777 (5)	0.99874 (14)	0.0730 (8)
O2	0.79909 (9)	0.1002 (6)	0.81382 (13)	0.0818 (8)
O3	1.07001 (10)	−0.5271 (7)	1.21363 (14)	0.0852 (9)
O4	1.01349 (9)	−0.3168 (7)	1.16428 (15)	0.0897 (10)
O5	0.22355 (8)	1.3185 (4)	−0.03675 (13)	0.0624 (7)
O6	0.04707 (8)	0.7561 (6)	−0.17868 (12)	0.0741 (8)
O7	0.32068 (10)	0.2884 (7)	0.22193 (14)	0.0894 (9)
O8	0.26593 (11)	0.4585 (7)	0.16330 (14)	0.0954 (10)
N1	0.98150 (9)	0.1336 (5)	0.99582 (14)	0.0511 (7)
H1	0.9759	−0.0309	0.9826	0.061*
N2	1.02079 (9)	0.1816 (6)	1.03432 (13)	0.0511 (7)
N3	1.05595 (10)	−0.3480 (6)	1.17783 (14)	0.0568 (7)
N4	0.23202 (9)	0.8791 (5)	−0.00297 (12)	0.0470 (6)
H4	0.2224	0.7104	−0.0057	0.056*

N5	0.27059 (9)	0.9449 (5)	0.03510 (12)	0.0465 (6)
N6	0.30788 (11)	0.4463 (6)	0.18136 (13)	0.0573 (7)
C1	0.75747 (14)	0.2779 (11)	0.8092 (2)	0.0971 (15)
H1A	0.7403	0.2803	0.8478	0.146*
H1B	0.7361	0.2112	0.7773	0.146*
H1C	0.7681	0.4617	0.7991	0.146*
C2	0.83484 (13)	0.1711 (8)	0.85484 (17)	0.0591 (9)
C3	0.87762 (14)	0.0170 (8)	0.85072 (19)	0.0692 (10)
H3	0.8807	−0.1200	0.8209	0.083*
C4	0.91548 (14)	0.0688 (7)	0.89123 (17)	0.0614 (9)
H4A	0.9440	−0.0352	0.8886	0.074*
C5	0.91161 (11)	0.2735 (6)	0.93575 (15)	0.0479 (8)
C6	0.86918 (12)	0.4255 (7)	0.93821 (17)	0.0575 (9)
H6	0.8663	0.5661	0.9673	0.069*
C7	0.83074 (13)	0.3740 (8)	0.89850 (17)	0.0639 (10)
H7	0.8021	0.4771	0.9014	0.077*
C8	0.95202 (11)	0.3410 (6)	0.97897 (15)	0.0493 (8)
C9	1.03790 (11)	−0.0312 (7)	1.06142 (15)	0.0475 (8)
H9	1.0226	−0.2017	1.0573	0.057*
C10	1.08216 (11)	−0.0030 (6)	1.09922 (14)	0.0452 (7)
C11	1.09264 (11)	−0.1602 (7)	1.15167 (15)	0.0476 (8)
C12	1.13661 (12)	−0.1393 (8)	1.18240 (17)	0.0619 (9)
H12	1.1428	−0.2501	1.2166	0.074*
C13	1.17137 (13)	0.0459 (9)	1.16240 (19)	0.0703 (11)
H13	1.2010	0.0622	1.1831	0.084*
C14	1.16188 (13)	0.2054 (8)	1.11180 (19)	0.0656 (10)
H14	1.1851	0.3327	1.0985	0.079*
C15	1.11838 (12)	0.1803 (7)	1.08016 (17)	0.0560 (9)
H15	1.1131	0.2883	1.0453	0.067*
C16	0.01518 (13)	0.5396 (9)	−0.1618 (2)	0.0761 (12)
H16A	0.0332	0.3696	−0.1594	0.114*
H16B	−0.0102	0.5224	−0.1922	0.114*
H16C	0.0009	0.5794	−0.1223	0.114*
C17	0.08517 (11)	0.8199 (7)	−0.14052 (16)	0.0506 (8)
C18	0.09396 (11)	0.7002 (7)	−0.08400 (16)	0.0525 (8)
H18	0.0729	0.5661	−0.0686	0.063*
C19	0.13441 (10)	0.7810 (7)	−0.05040 (15)	0.0491 (8)
H19	0.1406	0.6972	−0.0126	0.059*
C20	0.16590 (11)	0.9834 (6)	−0.07158 (14)	0.0435 (7)
C21	0.15563 (12)	1.1059 (7)	−0.12792 (15)	0.0544 (9)
H21	0.1758	1.2463	−0.1425	0.065*
C22	0.11605 (12)	1.0229 (8)	−0.16261 (16)	0.0593 (9)
H22	0.1101	1.1035	−0.2009	0.071*
C23	0.20924 (10)	1.0772 (6)	−0.03599 (15)	0.0451 (7)
C24	0.28988 (11)	0.7390 (7)	0.06273 (16)	0.0470 (7)
H24	0.2768	0.5626	0.0583	0.056*
C25	0.33316 (11)	0.7859 (6)	0.10178 (14)	0.0443 (7)
C26	0.34331 (11)	0.6392 (6)	0.15542 (15)	0.0467 (8)
C27	0.38649 (12)	0.6755 (8)	0.18840 (16)	0.0589 (9)

H27	0.3927	0.5705	0.2235	0.071*
C28	0.41980 (13)	0.8683 (8)	0.16846 (19)	0.0650 (10)
H28	0.4490	0.8939	0.1898	0.078*
C29	0.40985 (12)	1.0226 (8)	0.11709 (18)	0.0583 (9)
H29	0.4319	1.1580	0.1046	0.070*
C30	0.36755 (11)	0.9796 (7)	0.08357 (16)	0.0527 (8)
H30	0.3620	1.0829	0.0480	0.063*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0890 (17)	0.0340 (12)	0.0960 (19)	−0.0048 (11)	−0.0347 (16)	−0.0019 (13)
O2	0.0764 (17)	0.098 (2)	0.0704 (18)	−0.0061 (15)	−0.0289 (15)	0.0015 (16)
O3	0.0807 (17)	0.086 (2)	0.089 (2)	0.0083 (16)	0.0100 (16)	0.0312 (18)
O4	0.0496 (15)	0.114 (2)	0.106 (2)	−0.0133 (15)	−0.0068 (15)	0.040 (2)
O5	0.0674 (14)	0.0349 (11)	0.0847 (17)	−0.0063 (11)	−0.0201 (13)	0.0019 (12)
O6	0.0629 (15)	0.0995 (19)	0.0598 (16)	−0.0222 (14)	−0.0165 (13)	0.0047 (14)
O7	0.0940 (19)	0.093 (2)	0.082 (2)	0.0037 (18)	0.0064 (17)	0.0429 (18)
O8	0.0729 (19)	0.131 (2)	0.083 (2)	−0.0422 (18)	−0.0174 (16)	0.032 (2)
N1	0.0558 (16)	0.0365 (14)	0.0610 (17)	−0.0034 (12)	−0.0167 (14)	−0.0009 (13)
N2	0.0501 (15)	0.0481 (16)	0.0551 (16)	−0.0064 (12)	−0.0091 (14)	0.0029 (14)
N3	0.0526 (17)	0.0621 (19)	0.0559 (18)	0.0037 (14)	0.0037 (14)	0.0058 (17)
N4	0.0526 (14)	0.0322 (13)	0.0563 (16)	−0.0059 (11)	−0.0174 (14)	−0.0004 (12)
N5	0.0496 (15)	0.0406 (14)	0.0492 (15)	−0.0025 (12)	−0.0070 (13)	−0.0033 (13)
N6	0.0609 (19)	0.0612 (18)	0.0499 (17)	−0.0041 (15)	0.0006 (15)	0.0051 (16)
C1	0.053 (2)	0.151 (4)	0.087 (3)	0.003 (3)	−0.013 (2)	0.013 (3)
C2	0.060 (2)	0.067 (2)	0.050 (2)	−0.0104 (19)	−0.0114 (17)	0.0117 (19)
C3	0.086 (3)	0.059 (2)	0.063 (2)	0.012 (2)	−0.023 (2)	−0.0079 (19)
C4	0.073 (2)	0.049 (2)	0.062 (2)	0.0116 (18)	−0.0157 (19)	−0.0050 (18)
C5	0.0576 (19)	0.0326 (15)	0.053 (2)	−0.0017 (15)	−0.0086 (15)	0.0061 (15)
C6	0.061 (2)	0.054 (2)	0.058 (2)	0.0020 (17)	−0.0019 (18)	−0.0066 (17)
C7	0.055 (2)	0.078 (3)	0.059 (2)	0.0035 (19)	−0.0028 (18)	0.002 (2)
C8	0.0583 (19)	0.0366 (17)	0.053 (2)	−0.0057 (14)	−0.0072 (16)	0.0051 (15)
C9	0.0462 (17)	0.0418 (18)	0.0543 (19)	−0.0050 (14)	−0.0017 (15)	0.0008 (16)
C10	0.0418 (16)	0.0454 (17)	0.0485 (19)	−0.0002 (14)	−0.0006 (15)	−0.0027 (15)
C11	0.0411 (17)	0.0489 (19)	0.0527 (19)	−0.0004 (15)	−0.0028 (15)	−0.0055 (16)
C12	0.057 (2)	0.066 (2)	0.062 (2)	0.0022 (18)	−0.0077 (18)	−0.0009 (19)
C13	0.045 (2)	0.089 (3)	0.078 (3)	−0.011 (2)	−0.0144 (19)	−0.005 (2)
C14	0.053 (2)	0.074 (2)	0.070 (3)	−0.0181 (19)	−0.0002 (19)	−0.007 (2)
C15	0.0503 (19)	0.060 (2)	0.058 (2)	−0.0079 (16)	0.0022 (17)	0.0000 (17)
C16	0.052 (2)	0.085 (3)	0.091 (3)	−0.011 (2)	−0.012 (2)	−0.005 (2)
C17	0.0467 (18)	0.062 (2)	0.0436 (18)	−0.0023 (16)	−0.0065 (15)	−0.0039 (17)
C18	0.0504 (19)	0.051 (2)	0.056 (2)	−0.0097 (16)	0.0023 (17)	0.0049 (16)
C19	0.0513 (18)	0.0500 (18)	0.0461 (19)	−0.0035 (16)	−0.0069 (15)	0.0084 (15)
C20	0.0485 (17)	0.0347 (15)	0.0472 (18)	0.0015 (13)	−0.0025 (15)	−0.0014 (14)
C21	0.056 (2)	0.0516 (19)	0.056 (2)	−0.0057 (16)	−0.0042 (17)	0.0069 (17)
C22	0.062 (2)	0.069 (2)	0.047 (2)	−0.0058 (19)	−0.0112 (17)	0.0137 (18)
C23	0.0484 (17)	0.0362 (16)	0.0505 (19)	0.0017 (14)	−0.0049 (15)	−0.0007 (15)

C24	0.0481 (17)	0.0445 (18)	0.0483 (18)	−0.0054 (15)	−0.0048 (15)	−0.0032 (15)
C25	0.0457 (17)	0.0410 (17)	0.0462 (18)	0.0032 (14)	−0.0023 (15)	−0.0051 (15)
C26	0.0469 (17)	0.0485 (18)	0.0446 (18)	0.0020 (15)	−0.0028 (14)	−0.0037 (15)
C27	0.061 (2)	0.060 (2)	0.056 (2)	0.0060 (18)	−0.0153 (18)	0.0018 (18)
C28	0.0437 (18)	0.083 (3)	0.069 (2)	−0.0079 (19)	−0.0109 (18)	−0.010 (2)
C29	0.048 (2)	0.063 (2)	0.064 (2)	−0.0110 (17)	0.0025 (17)	−0.0041 (19)
C30	0.0527 (19)	0.053 (2)	0.0521 (19)	−0.0038 (16)	0.0004 (16)	0.0003 (16)

Geometric parameters (Å, °)

O1—C8	1.232 (4)	C10—C15	1.392 (4)
O2—C2	1.364 (4)	C10—C11	1.397 (5)
O2—C1	1.430 (5)	C11—C12	1.377 (5)
O3—N3	1.225 (4)	C12—C13	1.376 (5)
O4—N3	1.206 (4)	C12—H12	0.9300
O5—C23	1.232 (3)	C13—C14	1.365 (6)
O6—C17	1.365 (4)	C13—H13	0.9300
O6—C16	1.411 (5)	C14—C15	1.378 (5)
O7—N6	1.216 (4)	C14—H14	0.9300
O8—N6	1.213 (4)	C15—H15	0.9300
N1—C8	1.338 (4)	C16—H16A	0.9600
N1—N2	1.379 (3)	C16—H16B	0.9600
N1—H1	0.8600	C16—H16C	0.9600
N2—C9	1.274 (4)	C17—C18	1.376 (5)
N3—C11	1.467 (4)	C17—C22	1.381 (5)
N4—C23	1.348 (4)	C18—C19	1.380 (4)
N4—N5	1.376 (3)	C18—H18	0.9300
N4—H4	0.8600	C19—C20	1.382 (4)
N5—C24	1.276 (4)	C19—H19	0.9300
N6—C26	1.458 (4)	C20—C21	1.385 (4)
C1—H1A	0.9600	C20—C23	1.484 (4)
C1—H1B	0.9600	C21—C22	1.377 (5)
C1—H1C	0.9600	C21—H21	0.9300
C2—C7	1.368 (5)	C22—H22	0.9300
C2—C3	1.389 (5)	C24—C25	1.472 (4)
C3—C4	1.380 (5)	C24—H24	0.9300
C3—H3	0.9300	C25—C30	1.385 (4)
C4—C5	1.386 (5)	C25—C26	1.390 (4)
C4—H4A	0.9300	C26—C27	1.391 (4)
C5—C6	1.374 (4)	C27—C28	1.373 (5)
C5—C8	1.484 (4)	C27—H27	0.9300
C6—C7	1.380 (5)	C28—C29	1.367 (5)
C6—H6	0.9300	C28—H28	0.9300
C7—H7	0.9300	C29—C30	1.381 (5)
C9—C10	1.467 (4)	C29—H29	0.9300
C9—H9	0.9300	C30—H30	0.9300
C2—O2—C1	117.7 (3)	C14—C13—H13	120.3
C17—O6—C16	118.8 (3)	C12—C13—H13	120.3
C8—N1—N2	120.5 (3)	C13—C14—C15	120.9 (3)

C8—N1—H1	119.8	C13—C14—H14	119.6
N2—N1—H1	119.8	C15—C14—H14	119.6
C9—N2—N1	115.4 (3)	C14—C15—C10	121.5 (3)
O4—N3—O3	123.0 (3)	C14—C15—H15	119.3
O4—N3—C11	119.1 (3)	C10—C15—H15	119.3
O3—N3—C11	117.9 (3)	O6—C16—H16A	109.5
C23—N4—N5	120.5 (2)	O6—C16—H16B	109.5
C23—N4—H4	119.8	H16A—C16—H16B	109.5
N5—N4—H4	119.8	O6—C16—H16C	109.5
C24—N5—N4	114.6 (2)	H16A—C16—H16C	109.5
O8—N6—O7	122.4 (3)	H16B—C16—H16C	109.5
O8—N6—C26	118.2 (3)	O6—C17—C18	125.3 (3)
O7—N6—C26	119.3 (3)	O6—C17—C22	114.7 (3)
O2—C1—H1A	109.5	C18—C17—C22	120.1 (3)
O2—C1—H1B	109.5	C17—C18—C19	119.3 (3)
H1A—C1—H1B	109.5	C17—C18—H18	120.3
O2—C1—H1C	109.5	C19—C18—H18	120.3
H1A—C1—H1C	109.5	C18—C19—C20	121.6 (3)
H1B—C1—H1C	109.5	C18—C19—H19	119.2
O2—C2—C7	124.9 (3)	C20—C19—H19	119.2
O2—C2—C3	115.2 (4)	C19—C20—C21	118.0 (3)
C7—C2—C3	119.9 (3)	C19—C20—C23	122.8 (3)
C4—C3—C2	119.5 (4)	C21—C20—C23	119.2 (3)
C4—C3—H3	120.2	C22—C21—C20	121.0 (3)
C2—C3—H3	120.2	C22—C21—H21	119.5
C3—C4—C5	121.0 (4)	C20—C21—H21	119.5
C3—C4—H4A	119.5	C21—C22—C17	119.9 (3)
C5—C4—H4A	119.5	C21—C22—H22	120.1
C6—C5—C4	118.3 (3)	C17—C22—H22	120.1
C6—C5—C8	119.0 (3)	O5—C23—N4	122.3 (3)
C4—C5—C8	122.6 (3)	O5—C23—C20	122.4 (3)
C5—C6—C7	121.4 (3)	N4—C23—C20	115.3 (2)
C5—C6—H6	119.3	N5—C24—C25	118.8 (3)
C7—C6—H6	119.3	N5—C24—H24	120.6
C2—C7—C6	119.9 (3)	C25—C24—H24	120.6
C2—C7—H7	120.1	C30—C25—C26	116.6 (3)
C6—C7—H7	120.1	C30—C25—C24	119.1 (3)
O1—C8—N1	121.9 (3)	C26—C25—C24	124.2 (3)
O1—C8—C5	121.0 (3)	C25—C26—C27	122.3 (3)
N1—C8—C5	117.1 (3)	C25—C26—N6	121.1 (3)
N2—C9—C10	119.0 (3)	C27—C26—N6	116.5 (3)
N2—C9—H9	120.5	C28—C27—C26	119.1 (3)
C10—C9—H9	120.5	C28—C27—H27	120.4
C15—C10—C11	116.3 (3)	C26—C27—H27	120.4
C15—C10—C9	118.7 (3)	C29—C28—C27	119.7 (3)
C11—C10—C9	124.9 (3)	C29—C28—H28	120.2
C12—C11—C10	122.1 (3)	C27—C28—H28	120.2
C12—C11—N3	117.1 (3)	C28—C29—C30	120.8 (3)
C10—C11—N3	120.7 (3)	C28—C29—H29	119.6

C13—C12—C11	119.9 (3)	C30—C29—H29	119.6
C13—C12—H12	120.1	C29—C30—C25	121.4 (3)
C11—C12—H12	120.1	C29—C30—H30	119.3
C14—C13—C12	119.3 (3)	C25—C30—H30	119.3
C8—N1—N2—C9	160.9 (3)	C9—C10—C15—C14	−176.5 (3)
C23—N4—N5—C24	−178.3 (3)	C16—O6—C17—C18	−4.0 (5)
C1—O2—C2—C7	10.6 (5)	C16—O6—C17—C22	176.3 (3)
C1—O2—C2—C3	−170.4 (4)	O6—C17—C18—C19	179.0 (3)
O2—C2—C3—C4	−178.5 (4)	C22—C17—C18—C19	−1.3 (5)
C7—C2—C3—C4	0.6 (6)	C17—C18—C19—C20	1.2 (5)
C2—C3—C4—C5	−0.4 (6)	C18—C19—C20—C21	0.3 (5)
C3—C4—C5—C6	−0.5 (6)	C18—C19—C20—C23	179.1 (3)
C3—C4—C5—C8	−178.2 (3)	C19—C20—C21—C22	−1.8 (5)
C4—C5—C6—C7	1.3 (5)	C23—C20—C21—C22	179.4 (3)
C8—C5—C6—C7	179.1 (3)	C20—C21—C22—C17	1.8 (5)
O2—C2—C7—C6	179.1 (3)	O6—C17—C22—C21	179.6 (3)
C3—C2—C7—C6	0.2 (6)	C18—C17—C22—C21	−0.1 (5)
C5—C6—C7—C2	−1.1 (6)	N5—N4—C23—O5	4.7 (5)
N2—N1—C8—O1	−2.8 (5)	N5—N4—C23—C20	−175.6 (2)
N2—N1—C8—C5	178.0 (3)	C19—C20—C23—O5	−145.3 (3)
C6—C5—C8—O1	−28.7 (5)	C21—C20—C23—O5	33.4 (5)
C4—C5—C8—O1	149.0 (4)	C19—C20—C23—N4	35.0 (4)
C6—C5—C8—N1	150.6 (3)	C21—C20—C23—N4	−146.3 (3)
C4—C5—C8—N1	−31.8 (5)	N4—N5—C24—C25	176.6 (3)
N1—N2—C9—C10	175.0 (3)	N5—C24—C25—C30	−36.5 (4)
N2—C9—C10—C15	−35.7 (5)	N5—C24—C25—C26	146.2 (3)
N2—C9—C10—C11	148.7 (3)	C30—C25—C26—C27	−2.3 (4)
C15—C10—C11—C12	−1.1 (5)	C24—C25—C26—C27	175.0 (3)
C9—C10—C11—C12	174.7 (3)	C30—C25—C26—N6	175.1 (3)
C15—C10—C11—N3	176.4 (3)	C24—C25—C26—N6	−7.6 (5)
C9—C10—C11—N3	−7.8 (5)	O8—N6—C26—C25	−15.4 (5)
O4—N3—C11—C12	159.0 (3)	O7—N6—C26—C25	167.8 (3)
O3—N3—C11—C12	−19.7 (4)	O8—N6—C26—C27	162.2 (3)
O4—N3—C11—C10	−18.7 (5)	O7—N6—C26—C27	−14.6 (4)
O3—N3—C11—C10	162.7 (3)	C25—C26—C27—C28	1.9 (5)
C10—C11—C12—C13	1.6 (5)	N6—C26—C27—C28	−175.7 (3)
N3—C11—C12—C13	−176.0 (3)	C26—C27—C28—C29	0.6 (5)
C11—C12—C13—C14	−0.5 (6)	C27—C28—C29—C30	−2.5 (6)
C12—C13—C14—C15	−0.9 (6)	C28—C29—C30—C25	2.0 (6)
C13—C14—C15—C10	1.5 (6)	C26—C25—C30—C29	0.4 (5)
C11—C10—C15—C14	−0.5 (5)	C24—C25—C30—C29	−177.1 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.86	1.99	2.769 (3)	150
N4—H4···O5^{i}	0.86	2.01	2.819 (3)	156

Symmetry codes: (i) *x*, *y*−1, *z*.

Fig. 1

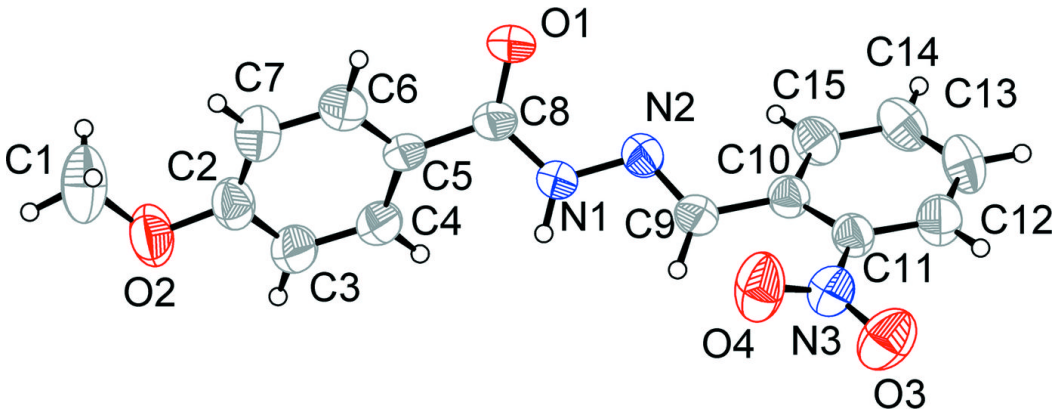
O1
C7
C6
C8
N2
C15
C14
C13
C1
C2
C5
C10
C4
N1
C9
C12
C11
O2
C3
O4
N3
O3

Fig. 2

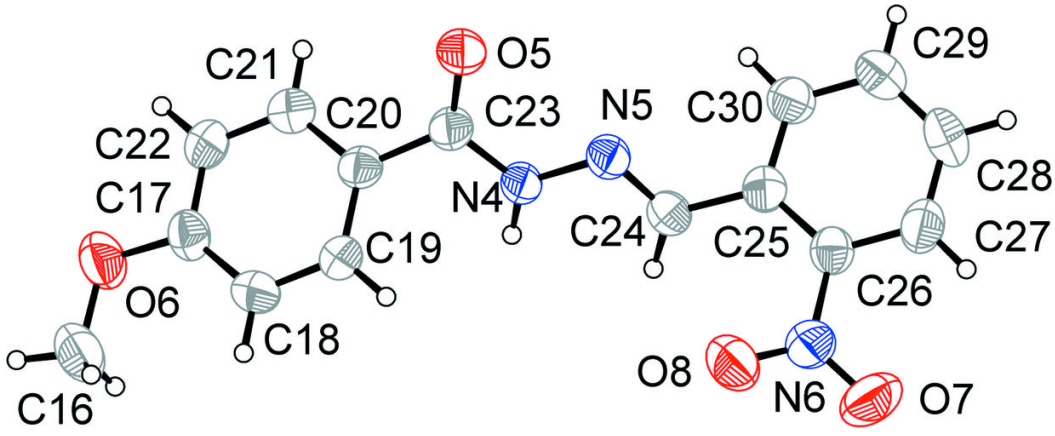
C21
O5
C20
C23
N5
C30
C29
C22
C28
C17
N4
C24
C25
C27
C19
O6
C26
C18
O8
N6
O7
C16

Fig. 3

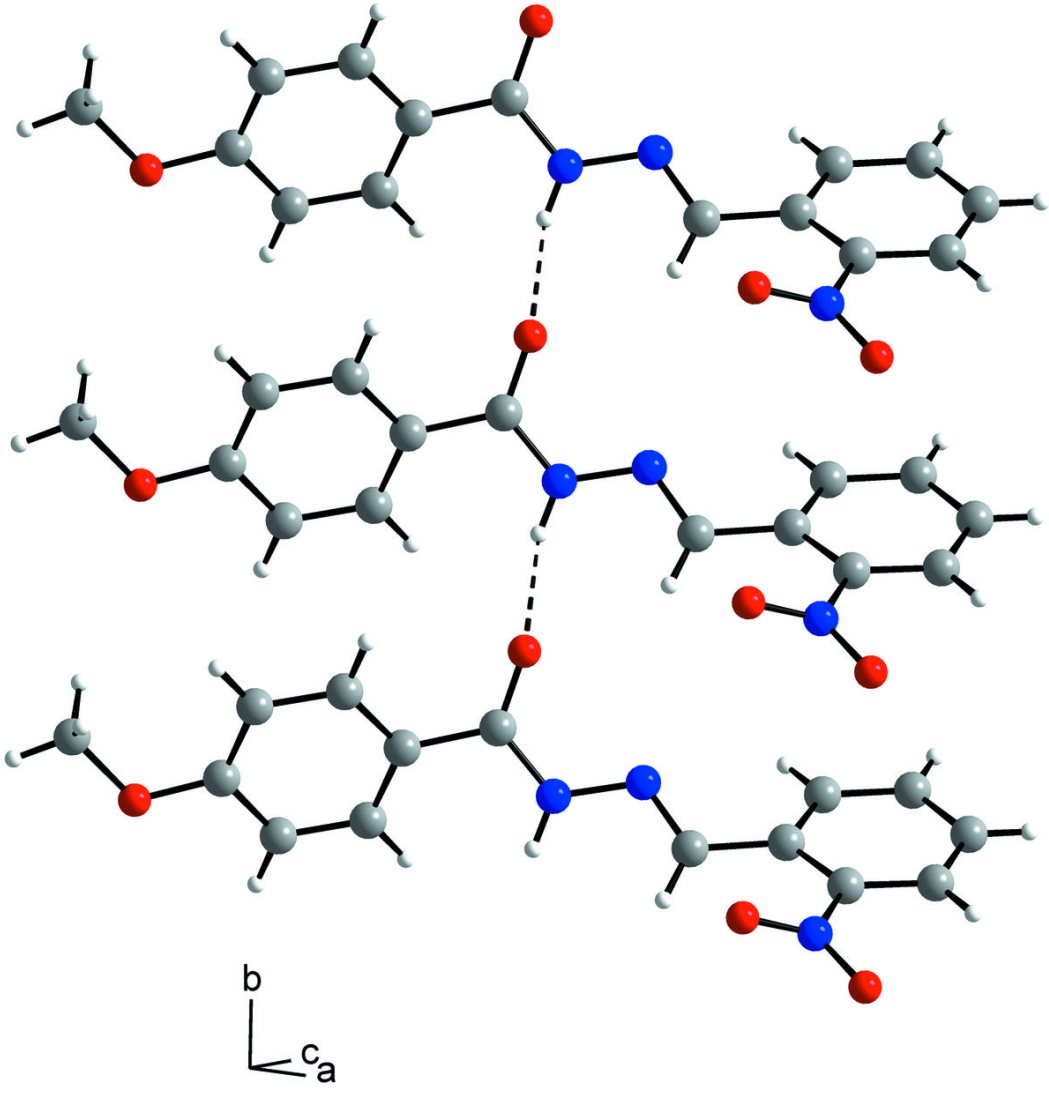

Fig. 4