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2′-[(5-Bromo-1*H*-indol-3-yl)methylene]-2-(1*H*-indol-3-yl)acetohydrazide ethyl acetate solvate

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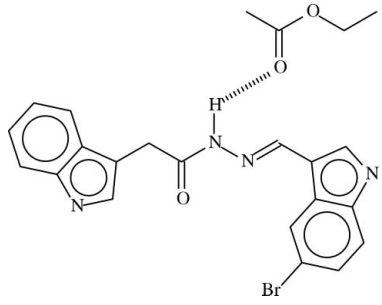
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.031; wR factor = 0.097; data-to-parameter ratio = 17.3.

The constituent molecules of the title compound, $C_{19}H_{15}BrN_4O\cdot C_4H_8O_2$, are linked by hydrogen bonds into a linear chain, with the acetohydrazide O atom serving as acceptor to the amide group as well as to the amino group of the bromoindole group. The ethyl acetate solvent molecule is also hydrogen bonded to the chain.

Related literature

For a related structure and background literature, see: Ali *et al.* (2007).



Experimental

Crystal data

$C_{19}H_{15}N_4OBr\cdot C_4H_8O_2$
M_r = 483.36
Monoclinic, $P2_1/c$
a = 11.9285 (2) Å
b = 12.8010 (2) Å
c = 15.5177 (3) Å
β = 110.665 (1)°
V = 2217.05 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.89 mm^{-1}
T = 173 (2) K
0.45 × 0.26 × 0.05 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.723, T_{max} = 0.911
34026 measured reflections
5100 independent reflections
4019 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.097
S = 1.08
5100 reflections
294 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*n*···O1^{i}	0.88 (1)	2.02 (1)	2.841 (2)	156 (2)
N2—H2^n···O2	0.88 (1)	2.02 (1)	2.893 (2)	171 (2)
N4—H4*n*···O1^{ii}	0.88 (1)	2.00 (1)	2.881 (2)	177 (3)

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

Data collection: *APEXII* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2384).

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supplementary materials

Acta Cryst. (2007). E**63**, o2731 [**doi:10.1107/S1600536807019824**]

2'-[(5-Bromo-1*H*-indol-3-yl)methylene]-2-(1*H*-indol-3-yl)acetohydrazide ethyl acetate solvate

H. M. Ali, J. Nazzatush Shimar and S. W. Ng

Comment

2'-[(5-Chloro-1*H*-indol-3-yl)methylene]-2-(1*H*-indol-3-yl)acetohydrazide adopts a three-dimensional hydrogen-bonded network structure in the solid state (Ali *et al.*, 2007). Replacing the chlorine atom by the heavier bromine atom furnishes the analogous molecule, but the compound crystallizes from ethyl acetate as the monosolvate (I) (Fig. 1). The Schff base adopts a chain structure arising from hydrogen bonds (Table 1); the solvent molecules are also hydrogen bonded to the chains.

Experimental

Indole-3-acetylhydrazine (0.3 g, 2 mmol) and 5-bromoindole-3-carboxaldehyde (0.4 g, 2 mmol) were dissolved in ethanol (100 ml). The reactants were heated under reflux for 1 h. The solvent was removed to give the Schiff base, which was purified by recrystallization from ethyl acetate to yield the title compound, (I), as a solvate.

Refinement

The carbon-bound H atoms were placed at calculated positions (C–H 0.95 to 0.99 Å), and they were included in the refinement in the riding model approximation with *U*(H) set to 1.2 timesU_{eq}(C). The nitrogen-bound H atoms were located in a difference Fourier map and were refined with a distance restraint (N–H = 0.88±0.01 Å); their U_{iso} values were freely refined.

Figures

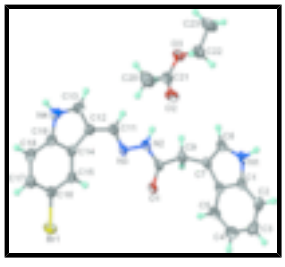


Fig. 1. View of the molecular structure of (I) with displacement ellipsoids drawn at the 70% probability level (H atoms are shown as spheres of arbitrary radius).

2'-[(5-Bromo-1*H*-indol-3-yl)methylene]-2-(1*H*-indol-\ 3-yl)acetohydrazide ethyl acetate solvate

Crystal data

$C_{19}H_{15}N_4OBr·C_4H_8O_2$	F_{000} = 992
M_r = 483.36	D_x = 1.448 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 5068 reflections
a = 11.9285 (2) Å	θ = 2.8–28.3°

b = 12.8010 (2) Å	μ = 1.89 mm^{-1}
c = 15.5177 (3) Å	T = 173 (2) K
β = 110.665 (1)º	Plate, colourless
V = 2217.05 (7) Å^3	0.45 × 0.26 × 0.05 mm
Z = 4	

Data collection

Bruker APEXII CCD diffractometer	5100 independent reflections
Radiation source: medium-focus sealed tube	4019 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.044
T = 173(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −15→15
T_{min} = 0.723, T_{max} = 0.911	k = −16→16
34026 measured reflections	l = −20→20

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.031	$w = 1/[\sigma^2(F_o^2) + (0.0523P)^2 + 0.4764P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.097	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.08	$\Delta\rho_{max}$ = 0.40 e Å^{-3}
5100 reflections	$\Delta\rho_{min}$ = −0.35 e Å^{-3}
294 parameters	Extinction correction: none
3 restraints	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	

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.

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

	x	y	z	U_{iso}*/U_{eq}
Br1	0.53417 (2)	0.232631 (19)	0.007875 (16)	0.03778 (10)
O1	0.82825 (13)	0.26073 (11)	0.42514 (9)	0.0248 (3)

O2	0.74889 (16)	0.55175 (13)	0.59819 (11)	0.0402 (4)
O3	0.78688 (14)	0.69909 (12)	0.68053 (10)	0.0311 (3)
N1	0.81936 (16)	0.20488 (15)	0.74199 (12)	0.0276 (4)
H1N	0.802 (2)	0.2053 (19)	0.7925 (11)	0.032 (6)*
N2	0.75052 (16)	0.41498 (13)	0.45022 (11)	0.0246 (4)
H2N	0.748 (2)	0.4622 (16)	0.4908 (14)	0.040 (7)*
N3	0.66752 (15)	0.42048 (13)	0.36088 (11)	0.0234 (4)
N4	0.35354 (17)	0.60494 (14)	0.15338 (13)	0.0309 (4)
H4N	0.3000 (18)	0.6535 (15)	0.1284 (17)	0.041 (7)*
C1	0.86676 (17)	0.12097 (16)	0.71193 (13)	0.0248 (4)
C2	0.87260 (19)	0.01600 (18)	0.73682 (15)	0.0321 (5)
H2	0.8393	−0.0081	0.7805	0.038*
C3	0.9284 (2)	−0.05150 (18)	0.69585 (16)	0.0367 (5)
H3	0.9332	−0.1236	0.7113	0.044*
C4	0.9783 (2)	−0.01653 (19)	0.63202 (16)	0.0361 (5)
H4	1.0183	−0.0648	0.6064	0.043*
C5	0.97030 (19)	0.08725 (17)	0.60547 (14)	0.0287 (5)
H5	1.0030	0.1101	0.5610	0.034*
C6	0.91329 (17)	0.15802 (16)	0.64522 (13)	0.0234 (4)
C7	0.88997 (18)	0.26799 (16)	0.63640 (13)	0.0226 (4)
C8	0.83429 (18)	0.29301 (17)	0.69700 (14)	0.0258 (4)
H8	0.8096	0.3613	0.7065	0.031*
C9	0.91793 (18)	0.34332 (16)	0.57291 (13)	0.0250 (4)
H9A	0.9991	0.3286	0.5722	0.030*
H9B	0.9178	0.4153	0.5961	0.030*
C10	0.82755 (17)	0.33558 (15)	0.47573 (13)	0.0218 (4)
C11	0.59448 (18)	0.49753 (15)	0.34742 (14)	0.0254 (4)
H11	0.5992	0.5412	0.3981	0.030*
C12	0.50573 (18)	0.52070 (15)	0.25894 (14)	0.0243 (4)
C13	0.4270 (2)	0.60308 (16)	0.24278 (15)	0.0304 (5)
H13	0.4245	0.6520	0.2881	0.036*
C14	0.47885 (17)	0.46777 (15)	0.17171 (14)	0.0224 (4)
C15	0.52562 (18)	0.38021 (15)	0.14205 (14)	0.0235 (4)
H15	0.5907	0.3419	0.1833	0.028*
C16	0.47385 (18)	0.35159 (16)	0.05091 (14)	0.0256 (4)
C17	0.37850 (19)	0.40635 (17)	−0.01250 (14)	0.0291 (5)
H17	0.3455	0.3835	−0.0747	0.035*
C18	0.33265 (19)	0.49350 (17)	0.01566 (15)	0.0300 (5)
H18	0.2687	0.5322	−0.0265	0.036*
C19	0.38279 (18)	0.52286 (16)	0.10744 (15)	0.0259 (4)
C20	0.8670 (3)	0.6856 (2)	0.56376 (19)	0.0478 (6)
H20A	0.8618	0.6422	0.5104	0.072*
H20B	0.9509	0.6907	0.6048	0.072*
H20C	0.8361	0.7556	0.5428	0.072*
C21	0.7946 (2)	0.63731 (18)	0.61433 (15)	0.0309 (5)
C22	0.7207 (2)	0.65917 (18)	0.73583 (15)	0.0327 (5)
H22A	0.7569	0.5933	0.7666	0.039*
H22B	0.6363	0.6454	0.6968	0.039*
C23	0.7271 (3)	0.7415 (2)	0.8057 (2)	0.0445 (6)

H23A	0.6880	0.7161	0.8476	0.067*
H23B	0.6864	0.8047	0.7744	0.067*
H23C	0.8112	0.7576	0.8409	0.067*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.04173 (16)	0.03789 (15)	0.03209 (14)	0.00672 (10)	0.01101 (10)	−0.00710 (9)
O1	0.0280 (8)	0.0282 (7)	0.0178 (7)	−0.0006 (6)	0.0074 (6)	−0.0008 (5)
O2	0.0530 (11)	0.0346 (9)	0.0346 (9)	−0.0034 (8)	0.0173 (8)	−0.0096 (7)
O3	0.0379 (9)	0.0315 (8)	0.0284 (8)	−0.0070 (7)	0.0172 (7)	−0.0053 (6)
N1	0.0278 (9)	0.0394 (10)	0.0174 (9)	−0.0011 (8)	0.0104 (7)	0.0004 (7)
N2	0.0292 (9)	0.0278 (9)	0.0147 (8)	−0.0018 (7)	0.0053 (7)	−0.0031 (7)
N3	0.0260 (9)	0.0274 (9)	0.0148 (8)	−0.0022 (7)	0.0049 (7)	0.0002 (6)
N4	0.0299 (10)	0.0277 (9)	0.0328 (10)	0.0088 (8)	0.0084 (8)	0.0046 (8)
C1	0.0193 (10)	0.0351 (11)	0.0163 (9)	−0.0011 (8)	0.0019 (8)	0.0019 (8)
C2	0.0283 (11)	0.0408 (12)	0.0221 (11)	0.0001 (10)	0.0028 (9)	0.0087 (9)
C3	0.0360 (13)	0.0322 (12)	0.0314 (12)	0.0041 (10)	−0.0012 (10)	0.0074 (9)
C4	0.0309 (12)	0.0392 (13)	0.0321 (12)	0.0087 (10)	0.0036 (10)	−0.0041 (10)
C5	0.0248 (10)	0.0381 (12)	0.0229 (10)	−0.0004 (9)	0.0080 (8)	−0.0042 (9)
C6	0.0192 (9)	0.0325 (10)	0.0151 (9)	−0.0012 (8)	0.0019 (7)	−0.0003 (8)
C7	0.0194 (9)	0.0306 (10)	0.0147 (9)	−0.0041 (8)	0.0020 (7)	−0.0025 (8)
C8	0.0233 (10)	0.0324 (11)	0.0191 (10)	−0.0009 (8)	0.0042 (8)	−0.0032 (8)
C9	0.0233 (10)	0.0316 (11)	0.0178 (9)	−0.0057 (8)	0.0044 (8)	−0.0007 (8)
C10	0.0240 (10)	0.0273 (10)	0.0157 (9)	−0.0071 (8)	0.0089 (8)	−0.0003 (7)
C11	0.0268 (10)	0.0279 (11)	0.0215 (10)	−0.0031 (8)	0.0087 (8)	−0.0024 (8)
C12	0.0237 (10)	0.0252 (9)	0.0242 (10)	−0.0015 (8)	0.0086 (8)	0.0006 (8)
C13	0.0332 (12)	0.0263 (10)	0.0323 (12)	0.0017 (9)	0.0124 (10)	−0.0003 (9)
C14	0.0205 (9)	0.0227 (9)	0.0232 (10)	−0.0022 (8)	0.0067 (8)	0.0036 (8)
C15	0.0198 (9)	0.0247 (10)	0.0244 (10)	0.0006 (8)	0.0059 (8)	0.0052 (8)
C16	0.0240 (10)	0.0273 (10)	0.0259 (10)	−0.0019 (8)	0.0092 (8)	−0.0005 (8)
C17	0.0249 (10)	0.0372 (12)	0.0216 (10)	−0.0025 (9)	0.0039 (8)	0.0006 (8)
C18	0.0231 (10)	0.0355 (12)	0.0263 (11)	0.0046 (9)	0.0024 (9)	0.0079 (9)
C19	0.0218 (10)	0.0275 (10)	0.0280 (11)	0.0020 (8)	0.0083 (8)	0.0056 (8)
C20	0.0534 (16)	0.0572 (17)	0.0437 (15)	−0.0050 (14)	0.0307 (13)	−0.0049 (13)
C21	0.0319 (11)	0.0349 (12)	0.0253 (11)	0.0036 (10)	0.0094 (9)	−0.0009 (9)
C22	0.0377 (12)	0.0347 (12)	0.0289 (11)	−0.0077 (10)	0.0157 (10)	−0.0023 (9)
C23	0.0434 (15)	0.0535 (16)	0.0462 (15)	−0.0113 (12)	0.0277 (13)	−0.0197 (12)

Geometric parameters (Å, °)

Br1—C16	1.903 (2)	C8—H8	0.9500
O1—C10	1.241 (2)	C9—C10	1.516 (3)
O2—C21	1.210 (3)	C9—H9A	0.9900
O3—C21	1.325 (3)	C9—H9B	0.9900
O3—C22	1.449 (3)	C11—C12	1.438 (3)
N1—C1	1.370 (3)	C11—H11	0.9500
N1—C8	1.371 (3)	C12—C13	1.375 (3)
N1—H1N	0.876 (10)	C12—C14	1.445 (3)

N2—C10	1.333 (3)	C13—H13	0.9500
N2—N3	1.392 (2)	C14—C15	1.400 (3)
N2—H2N	0.880 (10)	C14—C19	1.414 (3)
N3—C11	1.283 (3)	C15—C16	1.378 (3)
N4—C13	1.355 (3)	C15—H15	0.9500
N4—C19	1.382 (3)	C16—C17	1.401 (3)
N4—H4N	0.878 (10)	C17—C18	1.379 (3)
C1—C2	1.393 (3)	C17—H17	0.9500
C1—C6	1.418 (3)	C18—C19	1.388 (3)
C2—C3	1.376 (3)	C18—H18	0.9500
C2—H2	0.9500	C20—C21	1.491 (3)
C3—C4	1.397 (4)	C20—H20A	0.9800
C3—H3	0.9500	C20—H20B	0.9800
C4—C5	1.384 (3)	C20—H20C	0.9800
C4—H4	0.9500	C22—C23	1.494 (3)
C5—C6	1.400 (3)	C22—H22A	0.9900
C5—H5	0.9500	C22—H22B	0.9900
C6—C7	1.432 (3)	C23—H23A	0.9800
C7—C8	1.367 (3)	C23—H23B	0.9800
C7—C9	1.498 (3)	C23—H23C	0.9800
C21—O3—C22	116.75 (17)	C12—C11—H11	118.6
C1—N1—C8	109.18 (17)	C13—C12—C11	123.89 (19)
C1—N1—H1N	124.2 (16)	C13—C12—C14	106.10 (18)
C8—N1—H1N	124.3 (16)	C11—C12—C14	130.01 (18)
C10—N2—N3	120.51 (16)	N4—C13—C12	110.71 (19)
C10—N2—H2N	120.2 (17)	N4—C13—H13	124.6
N3—N2—H2N	119.2 (17)	C12—C13—H13	124.6
C11—N3—N2	113.85 (17)	C15—C14—C19	119.02 (19)
C13—N4—C19	108.97 (17)	C15—C14—C12	134.50 (18)
C13—N4—H4N	124.9 (17)	C19—C14—C12	106.48 (18)
C19—N4—H4N	126.0 (17)	C16—C15—C14	117.64 (18)
N1—C1—C2	130.4 (2)	C16—C15—H15	121.2
N1—C1—C6	107.53 (18)	C14—C15—H15	121.2
C2—C1—C6	122.1 (2)	C15—C16—C17	123.1 (2)
C3—C2—C1	117.6 (2)	C15—C16—Br1	119.00 (15)
C3—C2—H2	121.2	C17—C16—Br1	117.88 (16)
C1—C2—H2	121.2	C18—C17—C16	119.76 (19)
C2—C3—C4	121.5 (2)	C18—C17—H17	120.1
C2—C3—H3	119.2	C16—C17—H17	120.1
C4—C3—H3	119.2	C17—C18—C19	117.94 (19)
C5—C4—C3	121.1 (2)	C17—C18—H18	121.0
C5—C4—H4	119.4	C19—C18—H18	121.0
C3—C4—H4	119.4	N4—C19—C18	129.75 (19)
C4—C5—C6	118.9 (2)	N4—C19—C14	107.74 (18)
C4—C5—H5	120.6	C18—C19—C14	122.5 (2)
C6—C5—H5	120.6	C21—C20—H20A	109.5
C5—C6—C1	118.78 (19)	C21—C20—H20B	109.5
C5—C6—C7	134.60 (19)	H20A—C20—H20B	109.5
C1—C6—C7	106.60 (18)	C21—C20—H20C	109.5

C8—C7—C6	106.84 (18)	H20A—C20—H20C	109.5
C8—C7—C9	125.21 (19)	H20B—C20—H20C	109.5
C6—C7—C9	127.94 (18)	O2—C21—O3	123.5 (2)
C7—C8—N1	109.84 (19)	O2—C21—C20	124.7 (2)
C7—C8—H8	125.1	O3—C21—C20	111.9 (2)
N1—C8—H8	125.1	O3—C22—C23	106.35 (18)
C7—C9—C10	111.52 (16)	O3—C22—H22A	110.5
C7—C9—H9A	109.3	C23—C22—H22A	110.5
C10—C9—H9A	109.3	O3—C22—H22B	110.5
C7—C9—H9B	109.3	C23—C22—H22B	110.5
C10—C9—H9B	109.3	H22A—C22—H22B	108.6
H9A—C9—H9B	108.0	C22—C23—H23A	109.5
O1—C10—N2	123.97 (18)	C22—C23—H23B	109.5
O1—C10—C9	121.24 (18)	H23A—C23—H23B	109.5
N2—C10—C9	114.78 (17)	C22—C23—H23C	109.5
N3—C11—C12	122.86 (19)	H23A—C23—H23C	109.5
N3—C11—H11	118.6	H23B—C23—H23C	109.5
C10—N2—N3—C11	176.08 (18)	N3—C11—C12—C13	−179.6 (2)
C8—N1—C1—C2	−179.7 (2)	N3—C11—C12—C14	0.4 (3)
C8—N1—C1—C6	0.0 (2)	C19—N4—C13—C12	−0.3 (3)
N1—C1—C2—C3	−178.7 (2)	C11—C12—C13—N4	−179.56 (19)
C6—C1—C2—C3	1.6 (3)	C14—C12—C13—N4	0.4 (2)
C1—C2—C3—C4	0.4 (3)	C13—C12—C14—C15	179.9 (2)
C2—C3—C4—C5	−1.9 (3)	C11—C12—C14—C15	−0.1 (4)
C3—C4—C5—C6	1.4 (3)	C13—C12—C14—C19	−0.4 (2)
C4—C5—C6—C1	0.6 (3)	C11—C12—C14—C19	179.6 (2)
C4—C5—C6—C7	179.0 (2)	C19—C14—C15—C16	−0.7 (3)
N1—C1—C6—C5	178.16 (17)	C12—C14—C15—C16	179.0 (2)
C2—C1—C6—C5	−2.1 (3)	C14—C15—C16—C17	0.6 (3)
N1—C1—C6—C7	−0.6 (2)	C14—C15—C16—Br1	−179.69 (14)
C2—C1—C6—C7	179.09 (18)	C15—C16—C17—C18	0.2 (3)
C5—C6—C7—C8	−177.4 (2)	Br1—C16—C17—C18	−179.52 (16)
C1—C6—C7—C8	1.1 (2)	C16—C17—C18—C19	−0.8 (3)
C5—C6—C7—C9	3.5 (4)	C13—N4—C19—C18	−180.0 (2)
C1—C6—C7—C9	−178.03 (18)	C13—N4—C19—C14	0.1 (2)
C6—C7—C8—N1	−1.1 (2)	C17—C18—C19—N4	−179.2 (2)
C9—C7—C8—N1	178.00 (18)	C17—C18—C19—C14	0.8 (3)
C1—N1—C8—C7	0.7 (2)	C15—C14—C19—N4	180.00 (18)
C8—C7—C9—C10	−100.6 (2)	C12—C14—C19—N4	0.2 (2)
C6—C7—C9—C10	78.3 (3)	C15—C14—C19—C18	0.0 (3)
N3—N2—C10—O1	−3.1 (3)	C12—C14—C19—C18	−179.76 (19)
N3—N2—C10—C9	176.19 (16)	C22—O3—C21—O2	0.7 (3)
C7—C9—C10—O1	−74.1 (2)	C22—O3—C21—C20	−178.6 (2)
C7—C9—C10—N2	106.7 (2)	C21—O3—C22—C23	178.9 (2)
N2—N3—C11—C12	176.69 (18)		

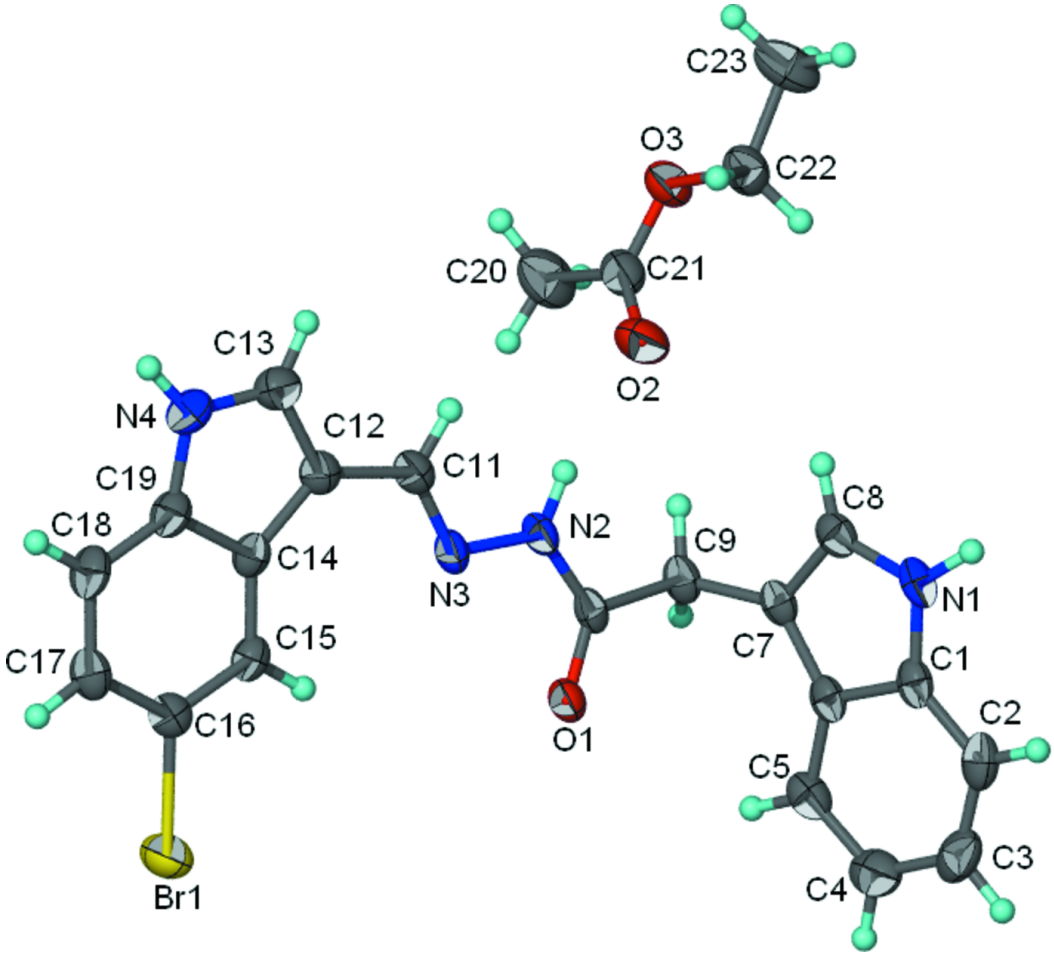
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

N1—H1n···O1^{i}	0.88 (1)	2.02 (1)	2.841 (2)	156 (2)
N2—H2n···O2	0.88 (1)	2.02 (1)	2.893 (2)	171 (2)
N4—H4n···O1^{ii}	0.88 (1)	2.00 (1)	2.881 (2)	177 (3)

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

Fig. 1


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