On the importance of antiparallel π–π interactions in the solid state of isatin-based hydrazides

Muhammad Naeem Ahmed,[a] Maryam Arif,[a] Farah Jabeen,[a] Haroon Ahmed Khan,[a] Khawaja Ansar Yasin[a], Muhammad Nawaz Tahir[b] , Antonio Franconetti[c] and Antonio Frontera[c*]

[a]Department of Chemistry, The University of Azad Jammu and Kashmir, Muzaffarabad, 13100, Pakistan

[b]Department of Physics, University of Sargodha, Sargodha, Pakistan

[c]Department de Quimica, Universitat de les Illes Balears, Crta. De Valldemossa km 7.5, 07122 Palma de Mallorca (Baleares), Spain

(*Z*)-*N*'-(2-oxo-1-propylindolin-3-ylidene) benzohydrazide (7)

Crystal data

$C_{18}H_{17}N_3O_2$	$F(000) = 648$
$M_r = 307.34$	$D_x = 1.289$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 7.167$ (2) Å	Cell parameters from 1636 reflections
$b = 24.911$ (9) Å	$\theta = 2.4$–$26.0°$
$c = 8.898$ (3) Å	$\mu = 0.09$ mm^{-1}
$\beta = 94.712$ (14)°	$T = 296$ K
$V = 1583.3$ (9) Å^3	Needle, yellow
$Z = 4$	0.40 × 0.25 × 0.22 mm

Data collection

Bruker Kappa APEXII CCD diffractometer	3095 independent reflections
Radiation source: fine-focus sealed tube	1636 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.060$
Detector resolution: 0.78 pixels mm^{-1}	$\theta_{max} = 26.0°$, $\theta_{min} = 2.4°$
ω scans	$h = -9 \rightarrow 9$
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)	$k = -32 \rightarrow 29$

T_{min} = 0.945, T_{max} = 0.975	l = −11→11
10341 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.061	Hydrogen site location: inferred from neighbouring sites
$wR(F^2)$ = 0.180	H-atom parameters constrained
S = 1.03	$w = 1/[\sigma^2(F_o^2) + (0.0817P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
3095 reflections	$(\Delta/\sigma)_{max} < 0.001$
208 parameters	$\Delta\rho_{max}$ = 0.35 e Å^{-3}
8 restraints	$\Delta\rho_{min}$ = −0.35 e Å^{-3}

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 Fset to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ 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}	Occ. (<1)
O1	0.3420 (3)	−0.15183 (8)	0.9647 (2)	0.0723 (6)	
O2	0.2846 (3)	0.03577 (8)	0.7714 (2)	0.0698 (6)	
N1	0.3133 (3)	−0.06587 (8)	0.8821 (2)	0.0530 (6)	
H1	0.3199	−0.0440	0.8079	0.064*	
N2	0.2753 (3)	−0.04694 (9)	1.0199 (2)	0.0504 (6)	
N3	0.2074 (3)	0.09248 (9)	0.9624 (3)	0.0624 (7)	
C1	0.3692 (3)	−0.13600 (10)	0.7031 (3)	0.0498 (7)	
C2	0.3705 (4)	−0.19004 (12)	0.6721 (4)	0.0773 (10)	
H2	0.3572	−0.2145	0.7495	0.093*	
C3	0.3912 (5)	−0.20876 (14)	0.5289 (4)	0.0952 (12)	
H3	0.3930	−0.2455	0.5105	0.114*	
C4	0.4091 (4)	−0.17338 (14)	0.4138 (4)	0.0806 (10)	
H4	0.4208	−0.1859	0.3166	0.097*	
C5	0.4097 (4)	−0.11936 (13)	0.4421 (4)	0.0735 (9)	

H5	0.4235	−0.0952	0.3641	0.088*	
C6	0.3901 (4)	−0.10063 (12)	0.5859 (3)	0.0627 (8)	
H6	0.3909	−0.0639	0.6042	0.075*	
C7	0.3412 (3)	−0.11997 (11)	0.8618 (3)	0.0525 (7)	
C8	0.2439 (3)	0.00398 (11)	1.0262 (3)	0.0453 (6)	
C9	0.1970 (3)	0.03353 (10)	1.1594 (3)	0.0471 (7)	
C10	0.1740 (4)	0.01892 (12)	1.3057 (3)	0.0624 (8)	
H10	0.1875	−0.0167	1.3360	0.075*	
C11	0.1305 (4)	0.05828 (15)	1.4074 (3)	0.0712 (9)	
H11	0.1151	0.0490	1.5069	0.085*	
C12	0.1097 (4)	0.11086 (14)	1.3628 (4)	0.0707 (9)	
H12	0.0807	0.1367	1.4326	0.085*	
C13	0.1312 (4)	0.12605 (12)	1.2162 (3)	0.0661 (8)	
H13	0.1160	0.1616	1.1859	0.079*	
C14	0.1758 (3)	0.08692 (11)	1.1160 (3)	0.0516 (7)	
C15	0.2481 (4)	0.04419 (11)	0.9028 (3)	0.0526 (7)	
C16A	0.2300 (6)	0.14386 (17)	0.8823 (5)	0.0781 (8)	0.806 (4)
H16A	0.3163	0.1388	0.8051	0.094*	0.806 (4)
H16B	0.2834	0.1704	0.9531	0.094*	0.806 (4)
C17A	0.0480 (5)	0.16412 (16)	0.8111 (5)	0.0781 (8)	0.806 (4)
H17A	−0.0406	0.1675	0.8873	0.094*	0.806 (4)
H17B	−0.0024	0.1385	0.7363	0.094*	0.806 (4)
C18A	0.0724 (6)	0.21806 (16)	0.7368 (5)	0.0781 (8)	0.806 (4)
H18A	0.1042	0.2446	0.8128	0.117*	0.806 (4)
H18B	−0.0423	0.2280	0.6804	0.117*	0.806 (4)
H18C	0.1707	0.2157	0.6701	0.117*	0.806 (4)
C16B	0.088 (2)	0.1350 (6)	0.865 (2)	0.0781 (8)	0.194 (4)
H16C	0.0594	0.1229	0.7617	0.094*	0.194 (4)
H16D	−0.0278	0.1439	0.9088	0.094*	0.194 (4)
C17B	0.222 (2)	0.1810 (6)	0.873 (2)	0.0781 (8)	0.194 (4)
H17C	0.3400	0.1680	0.8411	0.094*	0.194 (4)
H17D	0.2445	0.1910	0.9787	0.094*	0.194 (4)
C18B	0.171 (3)	0.2309 (6)	0.786 (2)	0.0781 (8)	0.194 (4)
H18D	0.0493	0.2428	0.8084	0.117*	0.194 (4)
H18E	0.1698	0.2234	0.6796	0.117*	0.194 (4)
H18F	0.2615	0.2584	0.8122	0.117*	0.194 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0973 (15)	0.0509 (13)	0.0695 (14)	0.0073 (10)	0.0119 (11)	0.0125 (12)
O2	0.1089 (15)	0.0593 (13)	0.0421 (12)	0.0024 (11)	0.0118 (10)	0.0045 (10)
N1	0.0690 (15)	0.0418 (13)	0.0488 (14)	0.0001 (10)	0.0076 (11)	0.0034 (11)
N2	0.0563 (13)	0.0478 (15)	0.0468 (14)	−0.0007 (10)	0.0027 (10)	0.0038 (11)
N3	0.0961 (17)	0.0426 (14)	0.0492 (15)	0.0101 (12)	0.0105 (12)	0.0077 (12)
C1	0.0457 (15)	0.0399 (16)	0.0640 (19)	0.0015 (11)	0.0059 (12)	0.0013 (14)

C2	0.114 (3)	0.0433 (19)	0.076 (2)	−0.0040 (16)	0.0137 (19)	0.0027 (17)
C3	0.152 (3)	0.051 (2)	0.085 (3)	−0.006 (2)	0.029 (2)	−0.016 (2)
C4	0.102 (2)	0.070 (2)	0.073 (2)	−0.0078 (18)	0.0259 (19)	−0.018 (2)
C5	0.090 (2)	0.063 (2)	0.072 (2)	0.0012 (16)	0.0329 (17)	0.0003 (18)
C6	0.0716 (18)	0.0458 (17)	0.074 (2)	0.0004 (13)	0.0252 (16)	−0.0023 (16)
C7	0.0513 (16)	0.0434 (17)	0.063 (2)	−0.0003 (12)	0.0047 (13)	0.0030 (15)
C8	0.0501 (15)	0.0433 (16)	0.0420 (15)	−0.0017 (11)	0.0002 (11)	0.0028 (12)
C9	0.0478 (15)	0.0505 (17)	0.0426 (15)	−0.0021 (12)	0.0017 (11)	0.0005 (13)
C10	0.0758 (19)	0.064 (2)	0.0472 (18)	0.0002 (15)	0.0046 (14)	0.0057 (16)
C11	0.078 (2)	0.094 (3)	0.0415 (17)	−0.0015 (18)	0.0054 (14)	−0.0039 (18)
C12	0.0692 (19)	0.081 (3)	0.062 (2)	0.0014 (16)	0.0042 (15)	−0.0193 (19)
C13	0.078 (2)	0.0577 (19)	0.062 (2)	0.0073 (15)	0.0014 (15)	−0.0065 (17)
C14	0.0585 (16)	0.0507 (18)	0.0450 (16)	0.0011 (12)	0.0005 (12)	−0.0014 (14)
C15	0.0674 (17)	0.0468 (17)	0.0429 (17)	0.0005 (13)	0.0007 (13)	0.0034 (14)
C16A	0.0822 (17)	0.0610 (16)	0.0899 (18)	0.0041 (13)	−0.0008 (13)	0.0212 (14)
C17A	0.0822 (17)	0.0610 (16)	0.0899 (18)	0.0041 (13)	−0.0008 (13)	0.0212 (14)
C18A	0.0822 (17)	0.0610 (16)	0.0899 (18)	0.0041 (13)	−0.0008 (13)	0.0212 (14)
C16B	0.0822 (17)	0.0610 (16)	0.0899 (18)	0.0041 (13)	−0.0008 (13)	0.0212 (14)
C17B	0.0822 (17)	0.0610 (16)	0.0899 (18)	0.0041 (13)	−0.0008 (13)	0.0212 (14)
C18B	0.0822 (17)	0.0610 (16)	0.0899 (18)	0.0041 (13)	−0.0008 (13)	0.0212 (14)

Geometric parameters (Å, º)

O1—C7	1.211 (3)	C10—C11	1.387 (4)
O2—C15	1.236 (3)	C10—H10	0.9300
N1—N2	1.362 (3)	C11—C12	1.373 (4)
N1—C7	1.377 (3)	C11—H11	0.9300
N1—H1	0.8600	C12—C13	1.379 (4)
N2—C8	1.290 (3)	C12—H12	0.9300
N3—C15	1.356 (3)	C13—C14	1.376 (4)
N3—C14	1.410 (3)	C13—H13	0.9300
N3—C16A	1.480 (4)	C16A—C17A	1.491 (5)
N3—C16B	1.579 (17)	C16A—H16A	0.9700
C1—C2	1.374 (4)	C16A—H16B	0.9700
C1—C6	1.383 (4)	C17A—C18A	1.514 (5)
C1—C7	1.496 (4)	C17A—H17A	0.9700
C2—C3	1.376 (4)	C17A—H17B	0.9700
C2—H2	0.9300	C18A—H18A	0.9600
C3—C4	1.365 (4)	C18A—H18B	0.9600
C3—H3	0.9300	C18A—H18C	0.9600
C4—C5	1.369 (4)	C16B—C17B	1.494 (16)
C4—H4	0.9300	C16B—H16C	0.9700
C5—C6	1.380 (4)	C16B—H16D	0.9700
C5—H5	0.9300	C17B—C18B	1.499 (15)
C6—H6	0.9300	C17B—H17C	0.9700
C8—C9	1.457 (3)	C17B—H17D	0.9700

C8—C15	1.489 (4)	C18B—H18D	0.9600
C9—C10	1.375 (3)	C18B—H18E	0.9600
C9—C14	1.390 (4)	C18B—H18F	0.9600
N2—N1—C7	120.0 (2)	C14—C13—C12	117.9 (3)
N2—N1—H1	120.0	C14—C13—H13	121.0
C7—N1—H1	120.0	C12—C13—H13	121.0
C8—N2—N1	115.4 (2)	C13—C14—C9	121.6 (3)
C15—N3—C14	110.4 (2)	C13—C14—N3	128.5 (3)
C15—N3—C16A	122.9 (3)	C9—C14—N3	109.9 (2)
C14—N3—C16A	125.7 (3)	O2—C15—N3	126.1 (3)
C15—N3—C16B	120.3 (7)	O2—C15—C8	127.0 (3)
C14—N3—C16B	118.5 (7)	N3—C15—C8	106.9 (2)
C2—C1—C6	118.0 (3)	N3—C16A—C17A	111.8 (3)
C2—C1—C7	117.0 (3)	N3—C16A—H16A	109.3
C6—C1—C7	124.9 (2)	C17A—C16A—H16A	109.3
C1—C2—C3	121.4 (3)	N3—C16A—H16B	109.3
C1—C2—H2	119.3	C17A—C16A—H16B	109.3
C3—C2—H2	119.3	H16A—C16A—H16B	107.9
C4—C3—C2	120.0 (3)	C16A—C17A—C18A	111.0 (4)
C4—C3—H3	120.0	C16A—C17A—H17A	109.4
C2—C3—H3	120.0	C18A—C17A—H17A	109.4
C3—C4—C5	119.7 (3)	C16A—C17A—H17B	109.4
C3—C4—H4	120.1	C18A—C17A—H17B	109.4
C5—C4—H4	120.1	H17A—C17A—H17B	108.0
C4—C5—C6	120.3 (3)	C17A—C18A—H18A	109.5
C4—C5—H5	119.9	C17A—C18A—H18B	109.5
C6—C5—H5	119.9	H18A—C18A—H18B	109.5
C5—C6—C1	120.6 (3)	C17A—C18A—H18C	109.5
C5—C6—H6	119.7	H18A—C18A—H18C	109.5
C1—C6—H6	119.7	H18B—C18A—H18C	109.5
O1—C7—N1	122.2 (3)	C17B—C16B—N3	99.6 (12)
O1—C7—C1	123.1 (2)	C17B—C16B—H16C	111.9
N1—C7—C1	114.7 (2)	N3—C16B—H16C	111.9
N2—C8—C9	125.8 (2)	C17B—C16B—H16D	111.9
N2—C8—C15	127.9 (2)	N3—C16B—H16D	111.9
C9—C8—C15	106.3 (2)	H16C—C16B—H16D	109.6
C10—C9—C14	119.9 (3)	C16B—C17B—C18B	118.7 (14)
C10—C9—C8	133.6 (3)	C16B—C17B—H17C	107.6
C14—C9—C8	106.5 (2)	C18B—C17B—H17C	107.6
C9—C10—C11	118.8 (3)	C16B—C17B—H17D	107.6
C9—C10—H10	120.6	C18B—C17B—H17D	107.6
C11—C10—H10	120.6	H17C—C17B—H17D	107.1
C12—C11—C10	120.7 (3)	C17B—C18B—H18D	109.5
C12—C11—H11	119.7	C17B—C18B—H18E	109.5
C10—C11—H11	119.7	H18D—C18B—H18E	109.5

C11—C12—C13	121.2 (3)	C17B—C18B—H18F	109.5
C11—C12—H12	119.4	H18D—C18B—H18F	109.5
C13—C12—H12	119.4	H18E—C18B—H18F	109.5
C7—N1—N2—C8	−177.3 (2)	C12—C13—C14—N3	−179.0 (3)
C6—C1—C2—C3	−0.3 (4)	C10—C9—C14—C13	−0.3 (4)
C7—C1—C2—C3	178.6 (3)	C8—C9—C14—C13	−179.9 (2)
C1—C2—C3—C4	−0.6 (5)	C10—C9—C14—N3	179.4 (2)
C2—C3—C4—C5	1.2 (5)	C8—C9—C14—N3	−0.1 (3)
C3—C4—C5—C6	−0.8 (5)	C15—N3—C14—C13	180.0 (3)
C4—C5—C6—C1	−0.1 (4)	C16A—N3—C14—C13	11.0 (5)
C2—C1—C6—C5	0.6 (4)	C16B—N3—C14—C13	−35.5 (7)
C7—C1—C6—C5	−178.1 (2)	C15—N3—C14—C9	0.3 (3)
N2—N1—C7—O1	−3.6 (4)	C16A—N3—C14—C9	−168.7 (3)
N2—N1—C7—C1	176.12 (19)	C16B—N3—C14—C9	144.7 (6)
C2—C1—C7—O1	8.8 (4)	C14—N3—C15—O2	−179.1 (2)
C6—C1—C7—O1	−172.4 (3)	C16A—N3—C15—O2	−9.8 (5)
C2—C1—C7—N1	−170.8 (2)	C16B—N3—C15—O2	37.1 (8)
C6—C1—C7—N1	7.9 (3)	C14—N3—C15—C8	−0.3 (3)
N1—N2—C8—C9	178.8 (2)	C16A—N3—C15—C8	169.1 (3)
N1—N2—C8—C15	−1.3 (4)	C16B—N3—C15—C8	−144.0 (7)
N2—C8—C9—C10	0.3 (4)	N2—C8—C15—O2	−0.8 (4)
C15—C8—C9—C10	−179.5 (3)	C9—C8—C15—O2	179.1 (2)
N2—C8—C9—C14	179.8 (2)	N2—C8—C15—N3	−179.6 (2)
C15—C8—C9—C14	−0.1 (2)	C9—C8—C15—N3	0.2 (3)
C14—C9—C10—C11	−0.2 (4)	C15—N3—C16A—C17A	100.5 (4)
C8—C9—C10—C11	179.2 (3)	C14—N3—C16A—C17A	−91.8 (4)
C9—C10—C11—C12	0.3 (4)	N3—C16A—C17A—C18A	177.1 (4)
C10—C11—C12—C13	0.1 (5)	C15—N3—C16B—C17B	−122.5 (11)
C11—C12—C13—C14	−0.6 (4)	C14—N3—C16B—C17B	96.6 (13)
C12—C13—C14—C9	0.7 (4)	N3—C16B—C17B—C18B	176.0 (15)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2	0.86	2.03	2.718 (3)	137
C17*A*—H17*A*···O1^{i}	0.97	2.65	3.578 (5)	160
C16*B*—H16*D*···O1^{i}	0.97	2.61	3.568 (18)	171

Symmetry code: (i) −x, −y, −z+2.

(*Z*)-3-methyl-*N*'-(2-oxo-1-propylindolin-3-ylidene)benzohydrazide **(8)**

Crystal data

$C_{19}H_{19}N_3O_2$	$Z = 2$
$M_r = 321.37$	$F(000) = 340$
Triclinic, $P\overline{1}$	$D_x = 1.272$ Mg m^{-3}
$a = 7.7416$ (13) Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 8.6214$ (17) Å	Cell parameters from 2288 reflections
$c = 13.993$ (2) Å	$\theta = 2.8$–$26.5°$
$\alpha = 98.324$ (5)°	$\mu = 0.08$ mm^{-1}
$\beta = 104.603$ (8)°	$T = 296$ K
$\gamma = 107.114$ (7)°	Needle, yellow
$V = 839.2$ (3) Å^3	0.38 × 0.23 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer	3408 independent reflections
Radiation source: fine-focus sealed tube	2288 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.047$
Detector resolution: 0.77 pixels mm^{-1}	$\theta_{max} = 26.5°$, $\theta_{min} = 2.8°$
ω scans	$h = -5 \rightarrow 9$
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)	$k = -10 \rightarrow 10$
$T_{min} = 0.885$, $T_{max} = 0.965$	$l = -17 \rightarrow 16$
9518 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.047$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.139$	H-atom parameters constrained
$S = 1.03$	$w = 1/[\sigma^2(F_o^2) + (0.0633P)^2 + 0.0561P]$ where $P = (F_o^2 + 2F_c^2)/3$
3408 reflections	$(\Delta/\sigma)_{max} < 0.001$
219 parameters	$\Delta\rho_{max} = 0.15$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.15$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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}
O1	0.1881 (2)	0.19859 (18)	0.35596 (11)	0.0852 (5)
O2	0.32723 (18)	0.36924 (14)	0.05092 (10)	0.0600 (4)
N1	0.2509 (2)	0.26660 (17)	0.21507 (11)	0.0547 (4)
H1	0.2840	0.3454	0.1850	0.066*
N2	0.22467 (19)	0.10776 (17)	0.16959 (11)	0.0496 (4)
N3	0.30677 (19)	0.14062 (16)	−0.06613 (11)	0.0476 (4)
C1	0.2488 (2)	0.4831 (2)	0.34503 (13)	0.0531 (5)
C2	0.2599 (3)	0.5360 (3)	0.44570 (15)	0.0653 (5)
H2	0.2545	0.4602	0.4869	0.078*
C3	0.2788 (3)	0.6992 (3)	0.48647 (15)	0.0672 (6)
C4	0.2882 (3)	0.8098 (3)	0.42395 (16)	0.0673 (6)
H4	0.3018	0.9198	0.4499	0.081*
C5	0.2778 (3)	0.7602 (2)	0.32419 (15)	0.0649 (5)
H5	0.2838	0.8364	0.2833	0.078*
C6	0.2584 (3)	0.5975 (2)	0.28447 (15)	0.0587 (5)
H6	0.2517	0.5645	0.2170	0.070*
C7	0.2891 (4)	0.7539 (3)	0.59578 (17)	0.1015 (9)
H7A	0.2631	0.6582	0.6245	0.152*
H7B	0.1966	0.8066	0.5988	0.152*
H7C	0.4140	0.8316	0.6335	0.152*
C8	0.2256 (3)	0.3042 (2)	0.30857 (14)	0.0581 (5)
C9	0.2457 (2)	0.08741 (19)	0.08033 (13)	0.0427 (4)
C10	0.2260 (2)	−0.06912 (19)	0.01599 (12)	0.0420 (4)
C11	0.1805 (2)	−0.2316 (2)	0.02661 (14)	0.0511 (4)
H11	0.1521	−0.2582	0.0843	0.061*
C12	0.1778 (3)	−0.3541 (2)	−0.04993 (15)	0.0603 (5)
H12	0.1485	−0.4640	−0.0435	0.072*
C13	0.2184 (3)	−0.3144 (2)	−0.13594 (15)	0.0605 (5)
H13	0.2165	−0.3984	−0.1865	0.073*
C14	0.2617 (2)	−0.1531 (2)	−0.14864 (14)	0.0541 (5)
H14	0.2879	−0.1271	−0.2069	0.065*
C15	0.2644 (2)	−0.03192 (19)	−0.07150 (13)	0.0436 (4)
C16	0.2978 (2)	0.2191 (2)	0.02309 (13)	0.0466 (4)
C17	0.3529 (2)	0.2230 (2)	−0.14538 (13)	0.0522 (4)
H17A	0.4321	0.1741	−0.1740	0.063*
H17B	0.4257	0.3403	−0.1150	0.063*

C18	0.1797 (3)	0.2082 (2)	−0.22943 (14)	0.0630 (5)
H18A	0.1083	0.2692	−0.2027	0.076*
H18B	0.0988	0.0918	−0.2547	0.076*
C19	0.2312 (3)	0.2759 (3)	−0.31660 (17)	0.0852 (7)
H19A	0.3168	0.3893	−0.2913	0.128*
H19B	0.1179	0.2720	−0.3662	0.128*
H19C	0.2913	0.2092	−0.3474	0.128*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.1358 (13)	0.0613 (9)	0.0621 (10)	0.0242 (9)	0.0458 (9)	0.0189 (8)
O2	0.0812 (9)	0.0360 (7)	0.0674 (9)	0.0187 (6)	0.0319 (7)	0.0137 (6)
N1	0.0725 (10)	0.0418 (9)	0.0509 (9)	0.0169 (7)	0.0262 (8)	0.0077 (7)
N2	0.0551 (8)	0.0433 (9)	0.0483 (9)	0.0138 (6)	0.0174 (7)	0.0092 (7)
N3	0.0595 (9)	0.0362 (8)	0.0479 (9)	0.0130 (6)	0.0210 (7)	0.0124 (6)
C1	0.0565 (10)	0.0527 (11)	0.0453 (10)	0.0153 (8)	0.0162 (8)	0.0039 (9)
C2	0.0767 (13)	0.0696 (14)	0.0480 (12)	0.0224 (10)	0.0228 (10)	0.0093 (10)
C3	0.0746 (13)	0.0710 (14)	0.0495 (12)	0.0238 (10)	0.0197 (10)	−0.0030 (11)
C4	0.0658 (12)	0.0588 (12)	0.0655 (14)	0.0178 (9)	0.0166 (10)	−0.0060 (11)
C5	0.0732 (13)	0.0580 (12)	0.0603 (13)	0.0204 (10)	0.0214 (10)	0.0082 (10)
C6	0.0688 (12)	0.0568 (12)	0.0466 (11)	0.0188 (9)	0.0194 (9)	0.0044 (9)
C7	0.140 (2)	0.101 (2)	0.0598 (15)	0.0421 (17)	0.0371 (15)	−0.0044 (14)
C8	0.0667 (12)	0.0576 (12)	0.0463 (11)	0.0145 (9)	0.0210 (9)	0.0102 (9)
C9	0.0424 (9)	0.0391 (9)	0.0454 (10)	0.0125 (7)	0.0131 (7)	0.0110 (7)
C10	0.0427 (9)	0.0376 (9)	0.0436 (9)	0.0129 (7)	0.0107 (7)	0.0101 (7)
C11	0.0600 (10)	0.0386 (10)	0.0540 (11)	0.0153 (8)	0.0161 (9)	0.0154 (8)
C12	0.0721 (12)	0.0363 (10)	0.0695 (13)	0.0187 (9)	0.0161 (10)	0.0139 (9)
C13	0.0714 (12)	0.0431 (11)	0.0621 (13)	0.0211 (9)	0.0172 (10)	0.0009 (9)
C14	0.0635 (11)	0.0488 (11)	0.0491 (11)	0.0180 (8)	0.0203 (9)	0.0075 (8)
C15	0.0454 (9)	0.0368 (9)	0.0457 (10)	0.0121 (7)	0.0123 (7)	0.0090 (7)
C16	0.0507 (10)	0.0371 (9)	0.0525 (11)	0.0144 (7)	0.0174 (8)	0.0115 (8)
C17	0.0602 (11)	0.0460 (10)	0.0523 (11)	0.0135 (8)	0.0231 (9)	0.0176 (8)
C18	0.0644 (12)	0.0649 (13)	0.0636 (13)	0.0204 (10)	0.0227 (10)	0.0265 (10)
C19	0.0817 (15)	0.117 (2)	0.0691 (15)	0.0367 (14)	0.0279 (12)	0.0473 (14)

Geometric parameters (Å, º)

O1—C8	1.212 (2)	C7—H7C	0.9600
O2—C16	1.2309 (18)	C9—C10	1.454 (2)
N1—N2	1.3566 (18)	C9—C16	1.500 (2)
N1—C8	1.378 (2)	C10—C11	1.380 (2)
N1—H1	0.8600	C10—C15	1.390 (2)
N2—C9	1.293 (2)	C11—C12	1.383 (2)
N3—C16	1.359 (2)	C11—H11	0.9300
N3—C15	1.4121 (19)	C12—C13	1.382 (3)

N3—C17	1.463 (2)	C12—H12	0.9300
C1—C6	1.388 (3)	C13—C14	1.381 (2)
C1—C2	1.389 (3)	C13—H13	0.9300
C1—C8	1.495 (3)	C14—C15	1.380 (2)
C2—C3	1.390 (3)	C14—H14	0.9300
C2—H2	0.9300	C17—C18	1.503 (2)
C3—C4	1.383 (3)	C17—H17A	0.9700
C3—C7	1.509 (3)	C17—H17B	0.9700
C4—C5	1.374 (3)	C18—C19	1.517 (3)
C4—H4	0.9300	C18—H18A	0.9700
C5—C6	1.381 (2)	C18—H18B	0.9700
C5—H5	0.9300	C19—H19A	0.9600
C6—H6	0.9300	C19—H19B	0.9600
C7—H7A	0.9600	C19—H19C	0.9600
C7—H7B	0.9600		
N2—N1—C8	121.29 (15)	C11—C10—C9	133.45 (16)
N2—N1—H1	119.4	C15—C10—C9	106.67 (14)
C8—N1—H1	119.4	C10—C11—C12	118.87 (17)
C9—N2—N1	115.50 (14)	C10—C11—H11	120.6
C16—N3—C15	110.25 (13)	C12—C11—H11	120.6
C16—N3—C17	124.88 (13)	C13—C12—C11	120.43 (17)
C15—N3—C17	124.87 (14)	C13—C12—H12	119.8
C6—C1—C2	118.69 (18)	C11—C12—H12	119.8
C6—C1—C8	124.06 (17)	C14—C13—C12	121.58 (17)
C2—C1—C8	117.25 (18)	C14—C13—H13	119.2
C1—C2—C3	121.7 (2)	C12—C13—H13	119.2
C1—C2—H2	119.2	C15—C14—C13	117.37 (17)
C3—C2—H2	119.2	C15—C14—H14	121.3
C4—C3—C2	118.05 (18)	C13—C14—H14	121.3
C4—C3—C7	121.1 (2)	C14—C15—C10	121.87 (15)
C2—C3—C7	120.9 (2)	C14—C15—N3	127.94 (15)
C5—C4—C3	121.24 (19)	C10—C15—N3	110.19 (14)
C5—C4—H4	119.4	O2—C16—N3	126.28 (15)
C3—C4—H4	119.4	O2—C16—C9	127.04 (16)
C4—C5—C6	120.2 (2)	N3—C16—C9	106.68 (13)
C4—C5—H5	119.9	N3—C17—C18	113.06 (14)
C6—C5—H5	119.9	N3—C17—H17A	109.0
C5—C6—C1	120.19 (18)	C18—C17—H17A	109.0
C5—C6—H6	119.9	N3—C17—H17B	109.0
C1—C6—H6	119.9	C18—C17—H17B	109.0
C3—C7—H7A	109.5	H17A—C17—H17B	107.8
C3—C7—H7B	109.5	C17—C18—C19	112.01 (16)
H7A—C7—H7B	109.5	C17—C18—H18A	109.2
C3—C7—H7C	109.5	C19—C18—H18A	109.2
H7A—C7—H7C	109.5	C17—C18—H18B	109.2

H7B—C7—H7C	109.5	C19—C18—H18B	109.2
O1—C8—N1	121.59 (18)	H18A—C18—H18B	107.9
O1—C8—C1	123.94 (17)	C18—C19—H19A	109.5
N1—C8—C1	114.47 (16)	C18—C19—H19B	109.5
N2—C9—C10	126.38 (15)	H19A—C19—H19B	109.5
N2—C9—C16	127.40 (15)	C18—C19—H19C	109.5
C10—C9—C16	106.22 (14)	H19A—C19—H19C	109.5
C11—C10—C15	119.87 (15)	H19B—C19—H19C	109.5
C8—N1—N2—C9	177.48 (15)	C10—C11—C12—C13	−0.6 (3)
C6—C1—C2—C3	0.5 (3)	C11—C12—C13—C14	−0.3 (3)
C8—C1—C2—C3	−179.09 (17)	C12—C13—C14—C15	0.5 (3)
C1—C2—C3—C4	−0.6 (3)	C13—C14—C15—C10	0.2 (2)
C1—C2—C3—C7	179.50 (19)	C13—C14—C15—N3	179.08 (15)
C2—C3—C4—C5	0.5 (3)	C11—C10—C15—C14	−1.1 (2)
C7—C3—C4—C5	−179.6 (2)	C9—C10—C15—C14	178.81 (14)
C3—C4—C5—C6	−0.3 (3)	C11—C10—C15—N3	179.84 (13)
C4—C5—C6—C1	0.2 (3)	C9—C10—C15—N3	−0.25 (17)
C2—C1—C6—C5	−0.3 (3)	C16—N3—C15—C14	−178.85 (16)
C8—C1—C6—C5	179.26 (17)	C17—N3—C15—C14	1.4 (3)
N2—N1—C8—O1	3.7 (3)	C16—N3—C15—C10	0.14 (18)
N2—N1—C8—C1	−176.52 (14)	C17—N3—C15—C10	−179.62 (14)
C6—C1—C8—O1	−168.18 (19)	C15—N3—C16—O2	179.96 (15)
C2—C1—C8—O1	11.3 (3)	C17—N3—C16—O2	−0.3 (3)
C6—C1—C8—N1	12.0 (3)	C15—N3—C16—C9	0.03 (17)
C2—C1—C8—N1	−168.48 (16)	C17—N3—C16—C9	179.80 (14)
N1—N2—C9—C10	179.83 (14)	N2—C9—C16—O2	−1.0 (3)
N1—N2—C9—C16	0.9 (2)	C10—C9—C16—O2	179.89 (15)
N2—C9—C10—C11	1.0 (3)	N2—C9—C16—N3	178.92 (15)
C16—C9—C10—C11	−179.85 (16)	C10—C9—C16—N3	−0.18 (17)
N2—C9—C10—C15	−178.86 (15)	C16—N3—C17—C18	−97.45 (19)
C16—C9—C10—C15	0.27 (17)	C15—N3—C17—C18	82.3 (2)
C15—C10—C11—C12	1.3 (2)	N3—C17—C18—C19	−173.06 (17)
C9—C10—C11—C12	−178.61 (17)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2	0.86	2.01	2.7154 (19)	138
C17—H17*B*···O2^{i}	0.97	2.53	3.482 (2)	167

Symmetry code: (i) −x, −y, −z+2.

(*Z*)-*N*'-(2-oxo-1-propylindolin-3-ylidene)-2-phenylacetohydrazide (9)

Crystal data

$C_{19}H_{19}N_3O_2$	$F(000) = 680$
$M_r = 321.37$	$D_x = 1.261$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 14.4085$ (13) Å	Cell parameters from 1824 reflections
$b = 7.0847$ (5) Å	$\theta = 3.0$–$26.0°$
$c = 17.8231$ (14) Å	$\mu = 0.08$ mm^{-1}
$\beta = 111.465$ (5)°	$T = 296$ K
$V = 1693.2$ (2) Å^3	Needle, yellow
$Z = 4$	0.42 × 0.20 × 0.16 mm

Data collection

Bruker Kappa APEXII CCD diffractometer	3317 independent reflections
Radiation source: fine-focus sealed tube	1824 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.048$
Detector resolution: 0.78 pixels mm^{-1}	$\theta_{max} = 26.0°$, $\theta_{min} = 3.0°$
ω scans	$h = -17 \rightarrow 16$
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)	$k = -8 \rightarrow 8$
$T_{min} = 0.949$, $T_{max} = 0.973$	$l = -19 \rightarrow 21$
8274 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.067$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.214$	H-atom parameters constrained
$S = 1.04$	$w = 1/[\sigma^2(F_o^2) + (0.0915P)^2 + 0.441P]$ where $P = (F_o^2 + 2F_c^2)/3$
3317 reflections	$(\Delta/\sigma)_{max} < 0.001$
176 parameters	$\Delta\rho_{max} = 0.38$ e Å^{-3}
8 restraints	$\Delta\rho_{min} = -0.31$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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}	Occ. (<1)
O1	0.3657 (2)	0.5820 (4)	0.40591 (18)	0.1057 (10)	
O2	0.04826 (17)	0.7060 (3)	0.30121 (13)	0.0716 (7)	
N1	0.2243 (2)	0.6352 (4)	0.42572 (16)	0.0658 (7)	
H1	0.1919	0.6463	0.3747	0.079*	
N2	0.17572 (19)	0.6584 (3)	0.47756 (14)	0.0543 (6)	
N3	−0.07288 (18)	0.7682 (3)	0.35454 (13)	0.0524 (6)	
C1A	0.3929 (4)	0.7412 (7)	0.5923 (3)	0.0719 (6)	0.534 (4)
C2A	0.3549 (4)	0.7424 (6)	0.6536 (3)	0.0719 (6)	0.534 (4)
H2A	0.3187	0.6396	0.6605	0.086*	0.534 (4)
C3A	0.3712 (4)	0.8972 (7)	0.7048 (3)	0.0719 (6)	0.534 (4)
H3A	0.3458	0.8981	0.7458	0.086*	0.534 (4)
C4A	0.4254 (3)	1.0508 (6)	0.6945 (3)	0.0719 (6)	0.534 (4)
H4A	0.4363	1.1544	0.7287	0.086*	0.534 (4)
C5A	0.4634 (3)	1.0496 (6)	0.6332 (3)	0.0719 (6)	0.534 (4)
H5A	0.4997	1.1524	0.6263	0.086*	0.534 (4)
C6A	0.4471 (4)	0.8948 (8)	0.5820 (3)	0.0719 (6)	0.534 (4)
H6A	0.4725	0.8939	0.5410	0.086*	0.534 (4)
C1B	0.3873 (5)	0.7558 (7)	0.5906 (3)	0.0719 (6)	0.466 (4)
C2B	0.3763 (5)	0.7779 (7)	0.6643 (4)	0.0719 (6)	0.466 (4)
H2B	0.3551	0.6770	0.6873	0.086*	0.466 (4)
C3B	0.3969 (5)	0.9510 (8)	0.7037 (3)	0.0719 (6)	0.466 (4)
H3B	0.3896	0.9658	0.7531	0.086*	0.466 (4)
C4B	0.4286 (4)	1.1019 (7)	0.6694 (3)	0.0719 (6)	0.466 (4)
H4B	0.4425	1.2177	0.6957	0.086*	0.466 (4)
C5B	0.4397 (4)	1.0798 (7)	0.5956 (3)	0.0719 (6)	0.466 (4)
H5B	0.4609	1.1808	0.5726	0.086*	0.466 (4)
C6B	0.4190 (4)	0.9068 (9)	0.5562 (3)	0.0719 (6)	0.466 (4)
H6B	0.4264	0.8920	0.5068	0.086*	0.466 (4)
C7	0.3748 (3)	0.5670 (4)	0.5430 (2)	0.0725 (10)	
H7A	0.3346	0.4821	0.5612	0.087*	
H7B	0.4384	0.5055	0.5531	0.087*	
C8	0.3241 (3)	0.5942 (5)	0.4537 (2)	0.0710 (9)	
C9	0.0828 (2)	0.7007 (3)	0.44586 (16)	0.0483 (7)	
C10	0.0170 (2)	0.7366 (3)	0.48969 (16)	0.0468 (7)	

C11	0.0326 (3)	0.7433 (4)	0.57080 (17)	0.0557 (8)	
H11	0.0950	0.7170	0.6095	0.067*	
C12	−0.0469 (3)	0.7903 (4)	0.59292 (19)	0.0633 (9)	
H12	−0.0380	0.7953	0.6473	0.076*	
C13	−0.1387 (3)	0.8295 (4)	0.5358 (2)	0.0646 (9)	
H13	−0.1910	0.8604	0.5523	0.078*	
C14	−0.1558 (2)	0.8244 (4)	0.45421 (19)	0.0577 (8)	
H14	−0.2182	0.8515	0.4158	0.069*	
C15	−0.0764 (2)	0.7774 (3)	0.43232 (16)	0.0472 (7)	
C16	0.0205 (2)	0.7236 (4)	0.35830 (18)	0.0529 (7)	
C17A	−0.1557 (3)	0.8064 (5)	0.2797 (2)	0.0804 (8)	0.534 (4)
H17A	−0.1326	0.8594	0.2395	0.096*	0.534 (4)
H17B	−0.2032	0.8925	0.2884	0.096*	0.534 (4)
C18A	−0.2039 (6)	0.6012 (11)	0.2533 (4)	0.0804 (8)	0.534 (4)
H18A	−0.1563	0.5190	0.2427	0.096*	0.534 (4)
H18B	−0.2209	0.5460	0.2964	0.096*	0.534 (4)
C19A	−0.2985 (5)	0.6203 (10)	0.1767 (3)	0.0804 (8)	0.534 (4)
H19A	−0.3276	0.4980	0.1606	0.121*	0.534 (4)
H19B	−0.3456	0.7009	0.1877	0.121*	0.534 (4)
H19C	−0.2811	0.6740	0.1341	0.121*	0.534 (4)
C17B	−0.1557 (3)	0.8064 (5)	0.2797 (2)	0.0804 (8)	0.466 (4)
H17C	−0.1281	0.8128	0.2377	0.096*	0.466 (4)
H17D	−0.1793	0.9323	0.2847	0.096*	0.466 (4)
C18B	−0.2444 (6)	0.6854 (12)	0.2489 (5)	0.0804 (8)	0.466 (4)
H18C	−0.2965	0.7481	0.2052	0.096*	0.466 (4)
H18D	−0.2694	0.6582	0.2914	0.096*	0.466 (4)
C19B	−0.2147 (6)	0.5092 (12)	0.2198 (5)	0.0804 (8)	0.466 (4)
H19D	−0.2713	0.4269	0.1992	0.121*	0.466 (4)
H19E	−0.1902	0.5378	0.1778	0.121*	0.466 (4)
H19F	−0.1632	0.4482	0.2636	0.121*	0.466 (4)

Atomic displacement parameters (Å²)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O1	0.0817 (19)	0.146 (3)	0.106 (2)	0.0129 (17)	0.0535 (18)	−0.0151 (18)
O2	0.0724 (15)	0.0996 (17)	0.0513 (13)	−0.0028 (12)	0.0327 (12)	−0.0069 (11)
N1	0.0583 (17)	0.0772 (17)	0.0648 (17)	0.0024 (13)	0.0257 (14)	−0.0082 (13)
N2	0.0560 (16)	0.0503 (13)	0.0591 (15)	0.0003 (12)	0.0242 (13)	−0.0035 (11)
N3	0.0551 (16)	0.0614 (14)	0.0404 (13)	−0.0037 (12)	0.0172 (11)	0.0003 (10)
C1A	0.0575 (12)	0.0798 (13)	0.0724 (12)	−0.0024 (9)	0.0166 (10)	0.0081 (10)
C2A	0.0575 (12)	0.0798 (13)	0.0724 (12)	−0.0024 (9)	0.0166 (10)	0.0081 (10)
C3A	0.0575 (12)	0.0798 (13)	0.0724 (12)	−0.0024 (9)	0.0166 (10)	0.0081 (10)
C4A	0.0575 (12)	0.0798 (13)	0.0724 (12)	−0.0024 (9)	0.0166 (10)	0.0081 (10)
C5A	0.0575 (12)	0.0798 (13)	0.0724 (12)	−0.0024 (9)	0.0166 (10)	0.0081 (10)
C6A	0.0575 (12)	0.0798 (13)	0.0724 (12)	−0.0024 (9)	0.0166 (10)	0.0081 (10)
C1B	0.0575 (12)	0.0798 (13)	0.0724 (12)	−0.0024 (9)	0.0166 (10)	0.0081 (10)

C2B	0.0575 (12)	0.0798 (13)	0.0724 (12)	−0.0024 (9)	0.0166 (10)	0.0081 (10)
C3B	0.0575 (12)	0.0798 (13)	0.0724 (12)	−0.0024 (9)	0.0166 (10)	0.0081 (10)
C4B	0.0575 (12)	0.0798 (13)	0.0724 (12)	−0.0024 (9)	0.0166 (10)	0.0081 (10)
C5B	0.0575 (12)	0.0798 (13)	0.0724 (12)	−0.0024 (9)	0.0166 (10)	0.0081 (10)
C6B	0.0575 (12)	0.0798 (13)	0.0724 (12)	−0.0024 (9)	0.0166 (10)	0.0081 (10)
C7	0.059 (2)	0.066 (2)	0.092 (3)	0.0103 (16)	0.027 (2)	0.0130 (17)
C8	0.061 (2)	0.067 (2)	0.092 (3)	0.0019 (17)	0.036 (2)	−0.0074 (18)
C9	0.0560 (19)	0.0422 (14)	0.0478 (16)	−0.0040 (13)	0.0202 (14)	−0.0043 (11)
C10	0.0565 (18)	0.0398 (14)	0.0438 (16)	−0.0048 (12)	0.0180 (14)	−0.0006 (11)
C11	0.068 (2)	0.0514 (16)	0.0472 (17)	−0.0056 (14)	0.0202 (15)	0.0018 (12)
C12	0.086 (3)	0.0634 (18)	0.0478 (18)	−0.0138 (17)	0.0337 (19)	−0.0016 (14)
C13	0.075 (2)	0.0637 (19)	0.070 (2)	−0.0089 (17)	0.044 (2)	−0.0076 (15)
C14	0.0560 (19)	0.0584 (17)	0.061 (2)	−0.0012 (14)	0.0247 (16)	0.0016 (14)
C15	0.0568 (18)	0.0428 (14)	0.0449 (16)	−0.0075 (13)	0.0221 (14)	−0.0022 (11)
C16	0.0570 (19)	0.0569 (17)	0.0480 (17)	−0.0052 (14)	0.0228 (15)	−0.0053 (13)
C17A	0.0647 (17)	0.111 (2)	0.0559 (15)	−0.0069 (14)	0.0110 (13)	−0.0056 (14)
C18A	0.0647 (17)	0.111 (2)	0.0559 (15)	−0.0069 (14)	0.0110 (13)	−0.0056 (14)
C19A	0.0647 (17)	0.111 (2)	0.0559 (15)	−0.0069 (14)	0.0110 (13)	−0.0056 (14)
C17B	0.0647 (17)	0.111 (2)	0.0559 (15)	−0.0069 (14)	0.0110 (13)	−0.0056 (14)
C18B	0.0647 (17)	0.111 (2)	0.0559 (15)	−0.0069 (14)	0.0110 (13)	−0.0056 (14)
C19B	0.0647 (17)	0.111 (2)	0.0559 (15)	−0.0069 (14)	0.0110 (13)	−0.0056 (14)

Geometric parameters (Å, º)

O1—C8	1.211 (4)	C7—C8	1.501 (5)
O2—C16	1.228 (3)	C7—H7A	0.9700
N1—N2	1.358 (3)	C7—H7B	0.9700
N1—C8	1.370 (4)	C9—C10	1.454 (4)
N1—H1	0.8600	C9—C16	1.497 (4)
N2—C9	1.284 (4)	C10—C11	1.380 (4)
N3—C16	1.360 (4)	C10—C15	1.390 (4)
N3—C15	1.407 (3)	C11—C12	1.382 (4)
N3—C17B	1.453 (4)	C11—H11	0.9300
N3—C17A	1.453 (4)	C12—C13	1.370 (5)
C1A—C2A	1.3900	C12—H12	0.9300
C1A—C6A	1.3900	C13—C14	1.384 (4)
C1A—C7	1.482 (5)	C13—H13	0.9300
C2A—C3A	1.3900	C14—C15	1.377 (4)
C2A—H2A	0.9300	C14—H14	0.9300
C3A—C4A	1.3900	C17A—C18A	1.606 (8)
C3A—H3A	0.9300	C17A—H17A	0.9700
C4A—C5A	1.3900	C17A—H17B	0.9700
C4A—H4A	0.9300	C18A—C19A	1.542 (8)
C5A—C6A	1.3900	C18A—H18A	0.9700
C5A—H5A	0.9300	C18A—H18B	0.9700
C6A—H6A	0.9300	C19A—H19A	0.9600

C1B—C2B	1.3900	C19A—H19B	0.9600
C1B—C6B	1.3900	C19A—H19C	0.9600
C1B—C7	1.559 (5)	C17B—C18B	1.468 (8)
C2B—C3B	1.3900	C17B—H17C	0.9700
C2B—H2B	0.9300	C17B—H17D	0.9700
C3B—C4B	1.3900	C18B—C19B	1.473 (11)
C3B—H3B	0.9300	C18B—H18C	0.9700
C4B—C5B	1.3900	C18B—H18D	0.9700
C4B—H4B	0.9300	C19B—H19D	0.9600
C5B—C6B	1.3900	C19B—H19E	0.9600
C5B—H5B	0.9300	C19B—H19F	0.9600
C6B—H6B	0.9300		
N2—N1—C8	120.8 (3)	C11—C10—C15	120.4 (3)
N2—N1—H1	119.6	C11—C10—C9	132.9 (3)
C8—N1—H1	119.6	C15—C10—C9	106.7 (2)
C9—N2—N1	116.3 (3)	C10—C11—C12	118.2 (3)
C16—N3—C15	110.7 (2)	C10—C11—H11	120.9
C16—N3—C17B	123.7 (3)	C12—C11—H11	120.9
C15—N3—C17B	125.6 (3)	C13—C12—C11	120.9 (3)
C16—N3—C17A	123.7 (3)	C13—C12—H12	119.6
C15—N3—C17A	125.6 (3)	C11—C12—H12	119.6
C2A—C1A—C6A	120.0	C12—C13—C14	121.8 (3)
C2A—C1A—C7	115.9 (4)	C12—C13—H13	119.1
C6A—C1A—C7	124.0 (4)	C14—C13—H13	119.1
C1A—C2A—C3A	120.0	C15—C14—C13	117.2 (3)
C1A—C2A—H2A	120.0	C15—C14—H14	121.4
C3A—C2A—H2A	120.0	C13—C14—H14	121.4
C4A—C3A—C2A	120.0	C14—C15—C10	121.5 (3)
C4A—C3A—H3A	120.0	C14—C15—N3	128.5 (3)
C2A—C3A—H3A	120.0	C10—C15—N3	109.9 (3)
C3A—C4A—C5A	120.0	O2—C16—N3	126.8 (3)
C3A—C4A—H4A	120.0	O2—C16—C9	126.9 (3)
C5A—C4A—H4A	120.0	N3—C16—C9	106.3 (3)
C6A—C5A—C4A	120.0	N3—C17A—C18A	102.9 (4)
C6A—C5A—H5A	120.0	N3—C17A—H17A	111.2
C4A—C5A—H5A	120.0	C18A—C17A—H17A	111.2
C5A—C6A—C1A	120.0	N3—C17A—H17B	111.2
C5A—C6A—H6A	120.0	C18A—C17A—H17B	111.2
C1A—C6A—H6A	120.0	H17A—C17A—H17B	109.1
C2B—C1B—C6B	120.0	C19A—C18A—C17A	109.1 (6)
C2B—C1B—C7	125.5 (4)	C19A—C18A—H18A	109.9
C6B—C1B—C7	114.3 (4)	C17A—C18A—H18A	109.9
C1B—C2B—C3B	120.0	C19A—C18A—H18B	109.9
C1B—C2B—H2B	120.0	C17A—C18A—H18B	109.9
C3B—C2B—H2B	120.0	H18A—C18A—H18B	108.3

C2B—C3B—C4B	120.0	C18A—C19A—H19A	109.5
C2B—C3B—H3B	120.0	C18A—C19A—H19B	109.5
C4B—C3B—H3B	120.0	H19A—C19A—H19B	109.5
C5B—C4B—C3B	120.0	C18A—C19A—H19C	109.5
C5B—C4B—H4B	120.0	H19A—C19A—H19C	109.5
C3B—C4B—H4B	120.0	H19B—C19A—H19C	109.5
C4B—C5B—C6B	120.0	N3—C17B—C18B	123.0 (4)
C4B—C5B—H5B	120.0	N3—C17B—H17C	106.6
C6B—C5B—H5B	120.0	C18B—C17B—H17C	106.6
C5B—C6B—C1B	120.0	N3—C17B—H17D	106.6
C5B—C6B—H6B	120.0	C18B—C17B—H17D	106.6
C1B—C6B—H6B	120.0	H17C—C17B—H17D	106.5
C1A—C7—C8	115.7 (3)	C17B—C18B—C19B	107.6 (7)
C8—C7—C1B	112.4 (3)	C17B—C18B—H18C	110.2
C1A—C7—H7A	108.4	C19B—C18B—H18C	110.2
C8—C7—H7A	108.4	C17B—C18B—H18D	110.2
C1A—C7—H7B	108.4	C19B—C18B—H18D	110.2
C8—C7—H7B	108.4	H18C—C18B—H18D	108.5
H7A—C7—H7B	107.4	C18B—C19B—H19D	109.5
O1—C8—N1	118.9 (4)	C18B—C19B—H19E	109.5
O1—C8—C7	124.2 (3)	H19D—C19B—H19E	109.5
N1—C8—C7	116.9 (3)	C18B—C19B—H19F	109.5
N2—C9—C10	125.7 (3)	H19D—C19B—H19F	109.5
N2—C9—C16	127.9 (3)	H19E—C19B—H19F	109.5
C10—C9—C16	106.4 (3)		
C8—N1—N2—C9	178.5 (3)	C15—C10—C11—C12	0.4 (4)
C6A—C1A—C2A—C3A	0.0	C9—C10—C11—C12	177.2 (3)
C7—C1A—C2A—C3A	177.8 (5)	C10—C11—C12—C13	−0.2 (4)
C1A—C2A—C3A—C4A	0.0	C11—C12—C13—C14	−0.1 (4)
C2A—C3A—C4A—C5A	0.0	C12—C13—C14—C15	0.2 (4)
C3A—C4A—C5A—C6A	0.0	C13—C14—C15—C10	0.1 (4)
C4A—C5A—C6A—C1A	0.0	C13—C14—C15—N3	−177.7 (3)
C2A—C1A—C6A—C5A	0.0	C11—C10—C15—C14	−0.3 (4)
C7—C1A—C6A—C5A	−177.6 (5)	C9—C10—C15—C14	−177.9 (2)
C6B—C1B—C2B—C3B	0.0	C11—C10—C15—N3	177.8 (2)
C7—C1B—C2B—C3B	175.0 (5)	C9—C10—C15—N3	0.2 (3)
C1B—C2B—C3B—C4B	0.0	C16—N3—C15—C14	177.6 (3)
C2B—C3B—C4B—C5B	0.0	C17B—N3—C15—C14	−0.6 (4)
C3B—C4B—C5B—C6B	0.0	C17A—N3—C15—C14	−0.6 (4)
C4B—C5B—C6B—C1B	0.0	C16—N3—C15—C10	−0.4 (3)
C2B—C1B—C6B—C5B	0.0	C17B—N3—C15—C10	−178.6 (3)
C7—C1B—C6B—C5B	−175.5 (5)	C17A—N3—C15—C10	−178.6 (3)
C2A—C1A—C7—C8	125.0 (3)	C15—N3—C16—O2	−179.5 (3)
C6A—C1A—C7—C8	−57.4 (5)	C17B—N3—C16—O2	−1.3 (5)
C2B—C1B—C7—C8	141.3 (4)	C17A—N3—C16—O2	−1.3 (5)

C6B—C1B—C7—C8	−43.4 (5)	C15—N3—C16—C9	0.4 (3)
N2—N1—C8—O1	−177.0 (3)	C17B—N3—C16—C9	178.6 (2)
N2—N1—C8—C7	3.0 (4)	C17A—N3—C16—C9	178.6 (2)
C1A—C7—C8—O1	106.2 (4)	N2—C9—C16—O2	−0.2 (5)
C1B—C7—C8—O1	108.4 (4)	C10—C9—C16—O2	179.7 (3)
C1A—C7—C8—N1	−73.8 (4)	N2—C9—C16—N3	179.9 (3)
C1B—C7—C8—N1	−71.7 (4)	C10—C9—C16—N3	−0.2 (3)
N1—N2—C9—C10	−178.4 (2)	C16—N3—C17A—C18A	89.6 (4)
N1—N2—C9—C16	1.4 (4)	C15—N3—C17A—C18A	−92.5 (4)
N2—C9—C10—C11	2.7 (4)	N3—C17A—C18A—C19A	176.2 (5)
C16—C9—C10—C11	−177.1 (3)	C16—N3—C17B—C18B	114.6 (5)
N2—C9—C10—C15	179.8 (3)	C15—N3—C17B—C18B	−67.5 (6)
C16—C9—C10—C15	0.0 (3)	N3—C17B—C18B—C19B	−72.1 (7)

Hydrogen-bond geometry (Å,º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2	0.86	2.01	2.7154 (19)	138
C17—H17*B*···O2^{i}	0.97	2.53	3.482 (2)	167

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

(*Z*)-2-bromo-*N*'-(2-oxo-1-propylindolin-3-ylidene)benzohydrazide **(10)**

$C_{18}H_{16}BrN_3O_2$	$F(000)$ = 784
M_r = 386.25	D_x = 1.507 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, λ = 0.71073 Å
a = 7.9365 (8) Å	Cell parameters from 2070 reflections
b = 19.667 (2) Å	θ = 2.1–27.1°
c = 10.9290 (12) Å	μ = 2.43 mm^{-1}
β = 93.512 (4)°	T = 296 K
V = 1702.7 (3) Å^3	Plate, orange
Z = 4	0.36 × 0.24 × 0.15 mm
Data collection	
Bruker Kappa APEXII CCD diffractometer	3754 independent reflections
Radiation source: fine-focus sealed tube	2070 reflections with $I > 2\sigma(I)$
Graphite monochromator	R_{int} = 0.056

Detector resolution: 0.76 pixels mm^{-1}	$\theta_{max} = 27.1°$, $\theta_{min} = 2.1°$
ω scans	$h = -10 \rightarrow 8$
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)	$k = -25 \rightarrow 23$
$T_{min} = 0.495$, $T_{max} = 0.740$	$l = -14 \rightarrow 13$
13928 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.051$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.134$	H-atom parameters constrained
$S = 1.01$	$w = 1/[\sigma^2(F_o^2) + (0.0612P)^2 + 0.2153P]$ where $P = (F_o^2 + 2F_c^2)/3$
3754 reflections	$(\Delta/\sigma)_{max} < 0.001$
218 parameters	$\Delta\rho_{max} = 0.46$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.49$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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	0.08013 (5)	0.19779 (3)	0.20041 (4)	0.0755 (2)
O1	0.3093 (3)	0.14438 (13)	0.6597 (2)	0.0595 (7)
O2	0.4466 (3)	0.29024 (13)	0.3725 (2)	0.0562 (7)
N1	0.2221 (4)	0.03220 (15)	0.6501 (3)	0.0526 (8)
N2	0.3711 (4)	0.11729 (14)	0.3922 (2)	0.0445 (7)
N3	0.3995 (4)	0.18260 (14)	0.4280 (3)	0.0496 (8)
H3	0.3995	0.1933	0.5043	0.059*
C1	0.2867 (4)	0.09095 (19)	0.6047 (3)	0.0472 (9)

C2	0.3219 (4)	0.07606 (17)	0.4737 (3)	0.0425 (8)
C3	0.2785 (4)	0.00524 (16)	0.4532 (3)	0.0433 (8)
C4	0.2837 (5)	−0.03664 (19)	0.3518 (3)	0.0589 (10)
H4	0.3258	−0.0208	0.2795	0.071*
C5	0.2252 (6)	−0.1024 (2)	0.3601 (4)	0.0725 (12)
H5	0.2279	−0.1312	0.2927	0.087*
C6	0.1631 (6)	−0.1258 (2)	0.4663 (4)	0.0746 (13)
H6	0.1227	−0.1702	0.4692	0.090*
C7	0.1588 (5)	−0.0851 (2)	0.5699 (4)	0.0663 (11)
H7	0.1186	−0.1015	0.6425	0.080*
C8	0.2168 (4)	−0.01951 (17)	0.5604 (3)	0.0480 (9)
C9	0.4281 (4)	0.2313 (2)	0.3428 (3)	0.0423 (8)
C10	0.4366 (4)	0.20857 (15)	0.2124 (3)	0.0392 (8)
C11	0.2970 (4)	0.19333 (16)	0.1372 (3)	0.0431 (8)
C12	0.3097 (5)	0.17753 (18)	0.0154 (3)	0.0542 (10)
H12	0.2137	0.1675	−0.0344	0.065*
C13	0.4665 (6)	0.17672 (19)	−0.0314 (4)	0.0646 (12)
H13	0.4765	0.1658	−0.1135	0.078*
C14	0.6077 (6)	0.19172 (19)	0.0412 (4)	0.0637 (11)
H14	0.7136	0.1907	0.0091	0.076*
C15	0.5920 (5)	0.20843 (17)	0.1624 (4)	0.0528 (9)
H15	0.6879	0.2198	0.2113	0.063*
C16	0.1662 (5)	0.0251 (2)	0.7747 (3)	0.0625 (11)
H16A	0.0652	−0.0028	0.7725	0.075*
H16B	0.1374	0.0696	0.8055	0.075*
C17	0.2985 (6)	−0.0063 (2)	0.8599 (4)	0.0733 (12)
H17A	0.3963	0.0233	0.8670	0.088*
H17B	0.3333	−0.0493	0.8261	0.088*
C18	0.2345 (6)	−0.0183 (3)	0.9868 (4)	0.0879 (15)
H18A	0.2001	0.0241	1.0206	0.132*
H18B	0.3231	−0.0379	1.0393	0.132*
H18C	0.1400	−0.0489	0.9804	0.132*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0417 (3)	0.1212 (5)	0.0637 (3)	−0.0020 (2)	0.00353 (19)	0.0090 (2)
O1	0.090 (2)	0.0472 (15)	0.0413 (14)	−0.0037 (14)	0.0055 (13)	−0.0029 (12)
O2	0.0717 (18)	0.0481 (16)	0.0486 (15)	−0.0107 (13)	0.0023 (12)	−0.0010 (12)
N1	0.076 (2)	0.0468 (18)	0.0360 (16)	−0.0011 (16)	0.0094 (15)	0.0022 (14)
N2	0.0552 (18)	0.0409 (17)	0.0370 (16)	0.0049 (14)	0.0003 (13)	0.0024 (13)
N3	0.069 (2)	0.0463 (18)	0.0332 (16)	−0.0030 (15)	0.0005 (14)	0.0026 (14)
C1	0.057 (2)	0.046 (2)	0.0384 (19)	0.0075 (19)	0.0025 (16)	0.0071 (18)
C2	0.047 (2)	0.043 (2)	0.0371 (18)	0.0054 (17)	−0.0005 (15)	0.0047 (16)
C3	0.049 (2)	0.041 (2)	0.0388 (19)	0.0058 (17)	−0.0025 (15)	0.0024 (16)
C4	0.075 (3)	0.054 (3)	0.047 (2)	0.006 (2)	0.0011 (19)	−0.0041 (19)

C5	0.092 (3)	0.056 (3)	0.069 (3)	0.000 (2)	0.000 (2)	−0.018 (2)
C6	0.091 (3)	0.041 (2)	0.091 (3)	−0.009 (2)	−0.003 (3)	0.000 (2)
C7	0.085 (3)	0.046 (2)	0.068 (3)	−0.006 (2)	0.009 (2)	0.010 (2)
C8	0.055 (2)	0.041 (2)	0.048 (2)	0.0014 (18)	0.0006 (17)	0.0044 (18)
C9	0.040 (2)	0.048 (2)	0.0387 (19)	−0.0044 (17)	−0.0021 (14)	0.0065 (18)
C10	0.044 (2)	0.0363 (18)	0.0382 (18)	0.0004 (16)	0.0059 (15)	0.0083 (15)
C11	0.043 (2)	0.045 (2)	0.0417 (19)	−0.0005 (16)	0.0047 (15)	0.0077 (16)
C12	0.070 (3)	0.050 (2)	0.041 (2)	0.003 (2)	−0.0037 (19)	−0.0010 (17)
C13	0.096 (4)	0.055 (2)	0.046 (2)	0.003 (2)	0.023 (2)	−0.0012 (19)
C14	0.062 (3)	0.063 (3)	0.069 (3)	−0.004 (2)	0.027 (2)	0.002 (2)
C15	0.045 (2)	0.053 (2)	0.061 (2)	−0.0074 (18)	0.0081 (18)	0.0019 (19)
C16	0.079 (3)	0.064 (3)	0.046 (2)	−0.001 (2)	0.015 (2)	0.0072 (19)
C17	0.080 (3)	0.089 (3)	0.051 (2)	0.011 (3)	0.006 (2)	0.008 (2)
C18	0.103 (4)	0.110 (4)	0.051 (3)	0.021 (3)	0.010 (2)	0.023 (3)

Geometric parameters (Å, º)

Br1—C11	1.895 (3)	C7—H7	0.9300
O1—C1	1.219 (4)	C9—C10	1.500 (5)
O2—C9	1.209 (4)	C10—C11	1.372 (5)
N1—C1	1.369 (4)	C10—C15	1.379 (5)
N1—C8	1.411 (4)	C11—C12	1.376 (5)
N1—C16	1.465 (4)	C12—C13	1.374 (5)
N2—C2	1.283 (4)	C12—H12	0.9300
N2—N3	1.358 (4)	C13—C14	1.365 (6)
N3—C9	1.365 (4)	C13—H13	0.9300
N3—H3	0.8600	C14—C15	1.378 (5)
C1—C2	1.504 (5)	C14—H14	0.9300
C2—C3	1.449 (5)	C15—H15	0.9300
C3—C4	1.384 (5)	C16—C17	1.494 (5)
C3—C8	1.385 (5)	C16—H16A	0.9700
C4—C5	1.380 (5)	C16—H16B	0.9700
C4—H4	0.9300	C17—C18	1.524 (6)
C5—C6	1.369 (6)	C17—H17A	0.9700
C5—H5	0.9300	C17—H17B	0.9700
C6—C7	1.389 (6)	C18—H18A	0.9600
C6—H6	0.9300	C18—H18B	0.9600
C7—C8	1.377 (5)	C18—H18C	0.9600
C1—N1—C8	110.6 (3)	C11—C10—C9	123.6 (3)
C1—N1—C16	123.9 (3)	C15—C10—C9	118.1 (3)
C8—N1—C16	125.4 (3)	C10—C11—C12	121.6 (3)
C2—N2—N3	116.7 (3)	C10—C11—Br1	119.3 (3)
N2—N3—C9	120.0 (3)	C12—C11—Br1	119.0 (3)
N2—N3—H3	120.0	C13—C12—C11	119.0 (4)
C9—N3—H3	120.0	C13—C12—H12	120.5

O1—C1—N1	126.6 (3)	C11—C12—H12	120.5
O1—C1—C2	127.4 (3)	C14—C13—C12	120.7 (4)
N1—C1—C2	106.0 (3)	C14—C13—H13	119.6
N2—C2—C3	125.4 (3)	C12—C13—H13	119.6
N2—C2—C1	128.3 (3)	C13—C14—C15	119.4 (4)
C3—C2—C1	106.1 (3)	C13—C14—H14	120.3
C4—C3—C8	119.8 (3)	C15—C14—H14	120.3
C4—C3—C2	132.6 (3)	C14—C15—C10	121.1 (3)
C8—C3—C2	107.5 (3)	C14—C15—H15	119.4
C5—C4—C3	118.6 (4)	C10—C15—H15	119.4
C5—C4—H4	120.7	N1—C16—C17	112.2 (3)
C3—C4—H4	120.7	N1—C16—H16A	109.2
C6—C5—C4	120.7 (4)	C17—C16—H16A	109.2
C6—C5—H5	119.6	N1—C16—H16B	109.2
C4—C5—H5	119.6	C17—C16—H16B	109.2
C5—C6—C7	121.7 (4)	H16A—C16—H16B	107.9
C5—C6—H6	119.1	C16—C17—C18	111.8 (4)
C7—C6—H6	119.1	C16—C17—H17A	109.3
C8—C7—C6	117.0 (4)	C18—C17—H17A	109.3
C8—C7—H7	121.5	C16—C17—H17B	109.3
C6—C7—H7	121.5	C18—C17—H17B	109.3
C7—C8—C3	122.1 (3)	H17A—C17—H17B	107.9
C7—C8—N1	128.3 (3)	C17—C18—H18A	109.5
C3—C8—N1	109.7 (3)	C17—C18—H18B	109.5
O2—C9—N3	120.8 (3)	H18A—C18—H18B	109.5
O2—C9—C10	121.9 (3)	C17—C18—H18C	109.5
N3—C9—C10	117.2 (3)	H18A—C18—H18C	109.5
C11—C10—C15	118.1 (3)	H18B—C18—H18C	109.5
C2—N2—N3—C9	−170.5 (3)	C2—C3—C8—N1	−1.3 (4)
C8—N1—C1—O1	−179.1 (3)	C1—N1—C8—C7	−179.2 (4)
C16—N1—C1—O1	1.2 (6)	C16—N1—C8—C7	0.5 (6)
C8—N1—C1—C2	1.4 (4)	C1—N1—C8—C3	−0.1 (4)
C16—N1—C1—C2	−178.3 (3)	C16—N1—C8—C3	179.6 (3)
N3—N2—C2—C3	177.4 (3)	N2—N3—C9—O2	176.9 (3)
N3—N2—C2—C1	1.7 (5)	N2—N3—C9—C10	−3.5 (4)
O1—C1—C2—N2	−5.3 (6)	O2—C9—C10—C11	−102.9 (4)
N1—C1—C2—N2	174.2 (3)	N3—C9—C10—C11	77.6 (4)
O1—C1—C2—C3	178.4 (3)	O2—C9—C10—C15	71.5 (4)
N1—C1—C2—C3	−2.1 (4)	N3—C9—C10—C15	−108.1 (3)
N2—C2—C3—C4	3.4 (6)	C15—C10—C11—C12	0.7 (5)
C1—C2—C3—C4	179.9 (4)	C9—C10—C11—C12	175.1 (3)
N2—C2—C3—C8	−174.4 (3)	C15—C10—C11—Br1	−176.6 (2)
C1—C2—C3—C8	2.1 (4)	C9—C10—C11—Br1	−2.3 (4)
C8—C3—C4—C5	0.6 (5)	C10—C11—C12—C13	0.3 (5)
C2—C3—C4—C5	−177.0 (4)	Br1—C11—C12—C13	177.7 (3)

C3—C4—C5—C6	0.0 (6)	C11—C12—C13—C14	−0.4 (6)
C4—C5—C6—C7	−1.0 (7)	C12—C13—C14—C15	−0.6 (6)
C5—C6—C7—C8	1.3 (6)	C13—C14—C15—C10	1.7 (6)
C6—C7—C8—C3	−0.6 (6)	C11—C10—C15—C14	−1.7 (5)
C6—C7—C8—N1	178.3 (4)	C9—C10—C15—C14	−176.4 (3)
C4—C3—C8—C7	−0.3 (5)	C1—N1—C16—C17	−97.5 (4)
C2—C3—C8—C7	177.8 (3)	C8—N1—C16—C17	82.8 (5)
C4—C3—C8—N1	−179.4 (3)	N1—C16—C17—C18	−175.7 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···O1	0.86	2.11	2.778 (4)	134
C7—H7···Br1^{i}	0.93	3.06	3.923 (4)	155
C12—H12···O2^{ii}	0.93	2.44	3.255 (5)	146

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

(*Z*)-*N*'-2-(furan-2-yl)-*N*'-(2-oxo-1-propylindolin-3-ylidene)acetohydrazide **(11)**

Crystal data

$C_{16}H_{15}N_3O_3$	$F(000) = 624$
$M_r = 297.31$	$D_x = 1.323$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 6.977$ (2) Å	Cell parameters from 1283 reflections
$b = 9.0505$ (12) Å	$\theta = 2.8–27.0°$
$c = 23.689$ (3) Å	$\mu = 0.09$ mm^{-1}
$\beta = 93.725$ (5)°	$T = 296$ K
$V = 1492.6$ (5) Å^3	Needle, yellow
$Z = 4$	0.42 × 0.18 × 0.16 mm

Data collection

Bruker Kappa APEXII CCD diffractometer	3241 independent reflections
Radiation source: fine-focus sealed tube	1283 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.081$
Detector resolution: 0.76 pixels mm^{-1}	$\theta_{max} = 27.0°$, $\theta_{min} = 2.8°$
ω scans	$h = -7 \rightarrow 8$
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)	$k = -11 \rightarrow 11$
$T_{min} = 0.939$, $T_{max} = 0.977$	$l = -30 \rightarrow 28$
11887 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.072$	H-atom parameters constrained
$wR(F^2) = 0.256$	$w = 1/[\sigma^2(F_o^2) + (0.1162P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$
3241 reflections	$\Delta\rho_{max} = 0.33$ e Å^{-3}
177 parameters	$\Delta\rho_{min} = -0.26$ e Å^{-3}
0 restraints	Extinction correction: *SHELXL2014*/7 (Sheldrick 2014, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.020 (7)

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 $F^2 > \sigma(F^2)$ 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}	Occ. (<1)
O1	0.7831 (4)	0.2591 (3)	−0.03173 (10)	0.0845 (9)	
O2	0.8942 (4)	0.4360 (4)	0.16788 (13)	0.1101 (11)	
N1	0.6945 (5)	0.4550 (3)	−0.09000 (13)	0.0743 (9)	
N2	0.7977 (4)	0.4991 (4)	0.05681 (14)	0.0712 (9)	
N3	0.8371 (4)	0.3616 (4)	0.07649 (12)	0.0736 (9)	
H3A	0.8349	0.2890	0.0530	0.088*	
C1	0.6702 (5)	0.6082 (4)	−0.08358 (15)	0.0623 (9)	
C2	0.6210 (6)	0.7114 (5)	−0.12382 (19)	0.0841 (12)	
H2	0.5957	0.6841	−0.1614	0.101*	
C3	0.6096 (6)	0.8569 (5)	−0.1077 (3)	0.1026 (15)	
H3	0.5760	0.9285	−0.1347	0.123*	

C4	0.6469 (7)	0.8979 (5)	−0.0523 (3)	0.1069 (17)	
H4	0.6404	0.9971	−0.0423	0.128*	
C5	0.6943 (6)	0.7929 (5)	−0.0109 (2)	0.0902 (13)	
H5	0.7182	0.8205	0.0268	0.108*	
C6	0.7051 (5)	0.6466 (4)	−0.02701 (16)	0.0646 (10)	
C7	0.7544 (5)	0.5111 (4)	0.00321 (15)	0.0608 (9)	
C8	0.7476 (5)	0.3905 (4)	−0.03988 (15)	0.0650 (10)	
C9	0.8809 (5)	0.3339 (5)	0.13341 (17)	0.0831 (12)	
O3A	0.9035 (8)	0.0699 (5)	0.10547 (16)	0.0888 (8)	0.559 (6)
C10A	0.9113 (5)	0.1775 (4)	0.14767 (14)	0.0888 (8)	0.559 (6)
C11A	0.9581 (9)	0.1080 (6)	0.19926 (19)	0.0888 (8)	0.559 (6)
H11A	0.9727	0.1540	0.2344	0.107*	0.559 (6)
C12A	0.9792 (10)	−0.0426 (7)	0.1890 (3)	0.0888 (8)	0.559 (6)
H12A	1.0104	−0.1147	0.2160	0.107*	0.559 (6)
C13A	0.9455 (9)	−0.0662 (6)	0.1310 (2)	0.0888 (8)	0.559 (6)
H13A	0.9501	−0.1568	0.1126	0.107*	0.559 (6)
O3B	0.9681 (9)	0.1694 (7)	0.2001 (2)	0.0888 (8)	0.441 (6)
C10B	0.9113 (5)	0.1775 (4)	0.14767 (14)	0.0888 (8)	0.441 (6)
C11B	0.8816 (16)	0.0595 (9)	0.1198 (3)	0.0888 (8)	0.441 (6)
H11B	0.8354	0.0481	0.0824	0.107*	0.441 (6)
C12B	0.9338 (12)	−0.0464 (9)	0.1583 (4)	0.0888 (8)	0.441 (6)
H12B	0.9331	−0.1478	0.1519	0.107*	0.441 (6)
C13B	0.9873 (12)	0.0215 (9)	0.2079 (3)	0.0888 (8)	0.441 (6)
H13B	1.0297	−0.0251	0.2414	0.107*	0.441 (6)
C14	0.6878 (6)	0.3769 (5)	−0.14548 (18)	0.0976 (14)	
H14A	0.7250	0.4449	−0.1745	0.117*	
H14B	0.7794	0.2962	−0.1434	0.117*	
C15	0.4981 (7)	0.3191 (6)	−0.1612 (2)	0.1227 (18)	
H15A	0.4038	0.3977	−0.1605	0.147*	
H15B	0.4648	0.2437	−0.1344	0.147*	
C16	0.4968 (8)	0.2523 (6)	−0.2214 (2)	0.141 (2)	
H16A	0.5008	0.3305	−0.2487	0.211*	
H16B	0.3820	0.1952	−0.2288	0.211*	
H16C	0.6070	0.1897	−0.2240	0.211*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.111 (2)	0.0624 (18)	0.0785 (19)	0.0025 (14)	−0.0042 (14)	−0.0074 (14)
O2	0.120 (3)	0.146 (3)	0.064 (2)	0.007 (2)	0.0005 (16)	−0.0203 (19)
N1	0.100 (2)	0.0619 (19)	0.060 (2)	0.0030 (15)	−0.0062 (15)	−0.0108 (15)
N2	0.065 (2)	0.082 (2)	0.067 (2)	−0.0077 (15)	0.0118 (15)	−0.0138 (17)
N3	0.073 (2)	0.095 (2)	0.054 (2)	−0.0008 (17)	0.0066 (14)	−0.0079 (17)
C1	0.064 (2)	0.058 (2)	0.065 (2)	−0.0041 (16)	0.0105 (16)	−0.0027 (19)
C2	0.088 (3)	0.077 (3)	0.088 (3)	0.002 (2)	0.014 (2)	0.008 (2)
C3	0.106 (4)	0.078 (3)	0.127 (5)	0.005 (2)	0.034 (3)	0.018 (3)

C4	0.114 (4)	0.057 (3)	0.154 (5)	−0.008 (2)	0.047 (3)	−0.002 (3)
C5	0.102 (3)	0.071 (3)	0.101 (3)	−0.011 (2)	0.032 (2)	−0.029 (3)
C6	0.063 (2)	0.058 (2)	0.075 (3)	−0.0070 (16)	0.0161 (17)	−0.0098 (19)
C7	0.055 (2)	0.073 (2)	0.055 (2)	−0.0088 (16)	0.0106 (15)	−0.0129 (19)
C8	0.070 (2)	0.060 (2)	0.065 (3)	−0.0057 (18)	0.0040 (17)	−0.0067 (19)
C9	0.052 (2)	0.142 (4)	0.056 (3)	−0.001 (2)	0.0068 (17)	−0.017 (3)
O3A	0.0928 (15)	0.1149 (19)	0.0583 (14)	0.0223 (13)	0.0004 (11)	0.0087 (13)
C10A	0.0928 (15)	0.1149 (19)	0.0583 (14)	0.0223 (13)	0.0004 (11)	0.0087 (13)
C11A	0.0928 (15)	0.1149 (19)	0.0583 (14)	0.0223 (13)	0.0004 (11)	0.0087 (13)
C12A	0.0928 (15)	0.1149 (19)	0.0583 (14)	0.0223 (13)	0.0004 (11)	0.0087 (13)
C13A	0.0928 (15)	0.1149 (19)	0.0583 (14)	0.0223 (13)	0.0004 (11)	0.0087 (13)
O3B	0.0928 (15)	0.1149 (19)	0.0583 (14)	0.0223 (13)	0.0004 (11)	0.0087 (13)
C10B	0.0928 (15)	0.1149 (19)	0.0583 (14)	0.0223 (13)	0.0004 (11)	0.0087 (13)
C11B	0.0928 (15)	0.1149 (19)	0.0583 (14)	0.0223 (13)	0.0004 (11)	0.0087 (13)
C12B	0.0928 (15)	0.1149 (19)	0.0583 (14)	0.0223 (13)	0.0004 (11)	0.0087 (13)
C13B	0.0928 (15)	0.1149 (19)	0.0583 (14)	0.0223 (13)	0.0004 (11)	0.0087 (13)
C14	0.109 (4)	0.096 (3)	0.086 (3)	0.002 (3)	−0.007 (2)	−0.019 (3)
C15	0.108 (4)	0.153 (5)	0.106 (4)	−0.016 (3)	0.000 (3)	−0.024 (3)
C16	0.144 (5)	0.187 (5)	0.089 (4)	−0.008 (4)	−0.011 (3)	−0.068 (4)

Geometric parameters (Å, º)

O1—C8	1.227 (4)	O3A—C13A	1.394 (4)
O2—C9	1.233 (5)	C10A—C11A	1.394 (4)
N1—C8	1.353 (4)	C11A—C12A	1.395 (4)
N1—C1	1.406 (4)	C11A—H11A	0.9300
N1—C14	1.490 (5)	C12A—C13A	1.395 (4)
N2—C7	1.290 (5)	C12A—H12A	0.9300
N2—N3	1.351 (4)	C13A—H13A	0.9300
N3—C9	1.386 (5)	O3B—C10B	1.280 (7)
N3—H3A	0.8600	O3B—C13B	1.357 (6)
C1—C2	1.363 (5)	C10B—C11B	1.266 (10)
C1—C6	1.391 (5)	C11B—C12B	1.356 (6)
C2—C3	1.375 (6)	C11B—H11B	0.9300
C2—H2	0.9300	C12B—C13B	1.357 (6)
C3—C4	1.372 (6)	C12B—H12B	0.9300
C3—H3	0.9300	C13B—H13B	0.9300
C4—C5	1.390 (6)	C14—C15	1.449 (6)
C4—H4	0.9300	C14—H14A	0.9700
C5—C6	1.382 (5)	C14—H14B	0.9700
C5—H5	0.9300	C15—C16	1.548 (6)
C6—C7	1.450 (5)	C15—H15A	0.9700
C7—C8	1.493 (5)	C15—H15B	0.9700
C9—C10B	1.467 (6)	C16—H16A	0.9600
C9—C10A	1.467 (6)	C16—H16B	0.9600
O3A—C10A	1.394 (4)	C16—H16C	0.9600

C8—N1—C1	111.0 (3)	C10A—C11A—C12A	108.0
C8—N1—C14	124.1 (3)	C10A—C11A—H11A	126.0
C1—N1—C14	124.5 (3)	C12A—C11A—H11A	126.0
C7—N2—N3	116.5 (3)	C11A—C12A—C13A	108.0
N2—N3—C9	121.9 (3)	C11A—C12A—H12A	126.0
N2—N3—H3A	119.0	C13A—C12A—H12A	126.0
C9—N3—H3A	119.0	O3A—C13A—C12A	108.0
C2—C1—C6	121.6 (3)	O3A—C13A—H13A	126.0
C2—C1—N1	128.8 (3)	C12A—C13A—H13A	126.0
C6—C1—N1	109.6 (3)	C10B—O3B—C13B	102.2 (4)
C1—C2—C3	118.6 (4)	C11B—C10B—O3B	119.1 (6)
C1—C2—H2	120.7	C11B—C10B—C9	132.7 (5)
C3—C2—H2	120.7	O3B—C10B—C9	108.0 (4)
C4—C3—C2	121.0 (4)	C10B—C11B—C12B	102.6 (3)
C4—C3—H3	119.5	C10B—C11B—H11B	128.7
C2—C3—H3	119.5	C12B—C11B—H11B	128.7
C3—C4—C5	120.8 (4)	C11B—C12B—C13B	108.0
C3—C4—H4	119.6	C11B—C12B—H12B	126.0
C5—C4—H4	119.6	C13B—C12B—H12B	126.0
C6—C5—C4	118.3 (4)	O3B—C13B—C12B	108.0
C6—C5—H5	120.8	O3B—C13B—H13B	126.0
C4—C5—H5	120.8	C12B—C13B—H13B	126.0
C5—C6—C1	119.8 (4)	C15—C14—N1	111.9 (4)
C5—C6—C7	133.6 (4)	C15—C14—H14A	109.2
C1—C6—C7	106.6 (3)	N1—C14—H14A	109.2
N2—C7—C6	126.1 (3)	C15—C14—H14B	109.2
N2—C7—C8	127.3 (3)	N1—C14—H14B	109.2
C6—C7—C8	106.5 (3)	H14A—C14—H14B	107.9
O1—C8—N1	126.7 (3)	C14—C15—C16	109.1 (4)
O1—C8—C7	127.1 (3)	C14—C15—H15A	109.9
N1—C8—C7	106.2 (3)	C16—C15—H15A	109.9
O2—C9—N3	120.8 (4)	C14—C15—H15B	109.9
O2—C9—C10B	124.5 (4)	C16—C15—H15B	109.9
N3—C9—C10B	114.7 (4)	H15A—C15—H15B	108.3
O2—C9—C10A	124.5 (4)	C15—C16—H16A	109.5
N3—C9—C10A	114.7 (4)	C15—C16—H16B	109.5
C10A—O3A—C13A	108.0	H16A—C16—H16B	109.5
O3A—C10A—C11A	108.0	C15—C16—H16C	109.5
O3A—C10A—C9	120.7 (3)	H16A—C16—H16C	109.5
C11A—C10A—C9	131.2 (3)	H16B—C16—H16C	109.5
C7—N2—N3—C9	−178.4 (3)	C6—C7—C8—N1	−1.1 (3)
C8—N1—C1—C2	178.8 (4)	N2—N3—C9—O2	−3.4 (5)
C14—N1—C1—C2	6.2 (6)	N2—N3—C9—C10B	177.4 (3)
C8—N1—C1—C6	−1.1 (4)	N2—N3—C9—C10A	177.4 (3)
C14—N1—C1—C6	−173.7 (3)	C13A—O3A—C10A—	0.0

		C11A	
C6—C1—C2—C3	1.2 (5)	C13A—O3A—C10A—C9	177.5 (4)
N1—C1—C2—C3	−178.6 (3)	O2—C9—C10A—O3A	−176.5 (4)
C1—C2—C3—C4	0.1 (6)	N3—C9—C10A—O3A	2.6 (5)
C2—C3—C4—C5	−1.0 (7)	O2—C9—C10A—C11A	0.4 (6)
C3—C4—C5—C6	0.8 (6)	N3—C9—C10A—C11A	179.5 (4)
C4—C5—C6—C1	0.5 (5)	O3A—C10A—C11A—C12A	0.0
C4—C5—C6—C7	178.0 (4)	C9—C10A—C11A—C12A	−177.2 (4)
C2—C1—C6—C5	−1.5 (5)	C10A—C11A—C12A—C13A	0.0
N1—C1—C6—C5	178.4 (3)	C10A—O3A—C13A—C12A	0.0
C2—C1—C6—C7	−179.6 (3)	C11A—C12A—C13A—O3A	0.0
N1—C1—C6—C7	0.3 (4)	C13B—O3B—C10B—C11B	3.0 (10)
N3—N2—C7—C6	179.3 (3)	C13B—O3B—C10B—C9	179.0 (4)
N3—N2—C7—C8	−1.7 (5)	O2—C9—C10B—C11B	170.0 (8)
C5—C6—C7—N2	2.0 (6)	N3—C9—C10B—C11B	−10.8 (10)
C1—C6—C7—N2	179.7 (3)	O2—C9—C10B—O3B	−5.2 (6)
C5—C6—C7—C8	−177.2 (4)	N3—C9—C10B—O3B	173.9 (4)
C1—C6—C7—C8	0.5 (3)	O3B—C10B—C11B—C12B	−3.0 (10)
C1—N1—C8—O1	−178.6 (3)	C9—C10B—C11B—C12B	−177.8 (5)
C14—N1—C8—O1	−6.0 (6)	C10B—C11B—C12B—C13B	1.6 (5)
C1—N1—C8—C7	1.4 (4)	C10B—O3B—C13B—C12B	−1.6 (5)
C14—N1—C8—C7	174.0 (3)	C11B—C12B—C13B—O3B	0.0
N2—C7—C8—O1	−0.4 (6)	C8—N1—C14—C15	94.0 (5)
C6—C7—C8—O1	178.8 (3)	C1—N1—C14—C15	−94.3 (5)
N2—C7—C8—N1	179.6 (3)	N1—C14—C15—C16	174.9 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···O1	0.86	2.03	2.729 (4)	137
C13*B*—H13*B*···O2^{i}	0.93	2.21	3.102 (6)	161
C15—H15*A*···O2^{ii}	0.97	2.56	3.517 (6)	168

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