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5,5-Diphenyl-3-propylimidazolidine-2,4-dione

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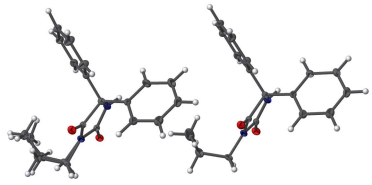
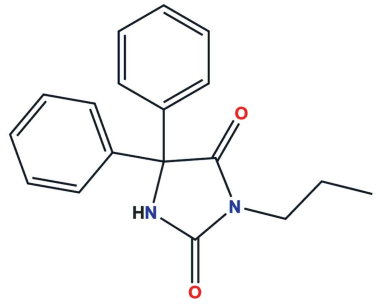
The asymmetric unit of the title compound, $C_{18}H_{18}N_2O_2$, consists of two independent molecules differing primarily in the orientation of the propyl substituent. One of the propyl groups is disordered over two positions with an occupancy ratio of 0.859 (2):0.141 (2). The two independent molecules are associated through a C—H···π(ring) interaction and sheets parallel to (011) are formed from further sets of C—H···π(ring) interactions. The sheets are connected *via* inversion-related N—H···O hydrogen bonds.

3D view



Chemical scheme



Structure description

In view of the broad spectrum of applications associated with hydantoïne and as a part of our ongoing work on such molecules (Ramli, Akrad *et al.*, 2017; Ramli, Guerrab *et al.*, 2017; Akrad *et al.*, 2017; Guerrab *et al.*, 2017*a*,*b*,*c*), we report herein on the synthesis and crystal structure of the title compound.

The asymmetric unit of the title compound consists of two independent molecules (Fig. 1) which differ in the orientations of the propyl groups, one of which is disordered over two sites [at N3, occupancy ratio 0.859 (2):0.141 (2)], and the phenyl rings. Thus the N1—C4—C5—C6 torsion angle is 58.11 (14)° while the N3—C22—C23—C24 torsion angle is −57.2 (2)°. Each imidazolidine-2,4-dione ring has two phenyl rings attached at the 5-position. The C7–C12 and C13–C18 phenyl rings are inclined to the C1/C2/N1/C3/N2 ring by 67.13 (6) and 66.09 (6)°, respectively, while the C25–C30 and C31–C36 phenyl rings are inclined to the C19/C20/N3/C21/N4 ring by 71.25 (6) and 64.48 (6)°, respectively.

In the crystal, C—H···π(ring) interactions (C5—H5*A*···*Cg*5, C15—H15···*Cg*2, C23—H23*A*···*Cg*2, C24—H24*C*···*Cg*6 and C35—H35···*Cg*5; Table 1) form layers parallel to (011) (Fig. 2; *Cg*2, *Cg*5 and *Cg*6 are the centroids of the C25–C30, C7–C12 and C13–C18 phenyl rings, respectively). These are connected in the direction of the diagonal of the *bc*

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

*Cg*2, *Cg*5 and *Cg*6 are the centroids of the C25–C30, C7–C12 and C13–C18 phenyl rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O4^{i}	0.908 (14)	1.915 (15)	2.8211 (11)	174.8 (12)
N4—H4···O2^{i}	0.913 (14)	1.917 (14)	2.8293 (10)	177.3 (12)
C5—H5*A*···*Cg*5^{ii}	1.033 (15)	2.651 (15)	3.6101 (13)	154.4 (11)
C15—H15···*Cg*2^{iii}	0.971 (15)	2.925 (14)	3.8055 (12)	154.1 (12)
C23—H23*A*···*Cg*2^{ii}	0.99	2.92	3.8118 (15)	151
C24—H24*C*···*Cg*6^{iv}	0.98	2.91	3.6320 (13)	131
C35—H35···*Cg*5	0.981 (15)	2.741 (15)	3.6627 (13)	156.9 (13)

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

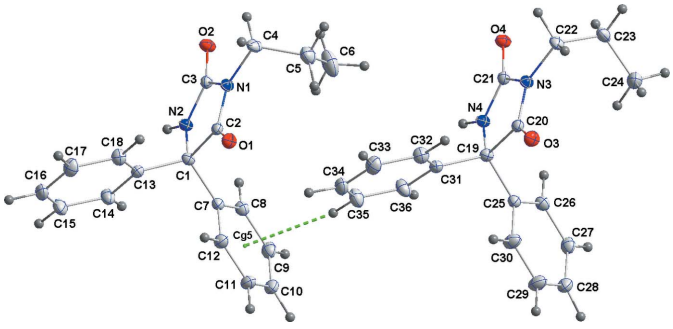


Figure 1
The asymmetric unit with labeling scheme and 50% probability ellipsoids. The C—H···π(ring) interaction is shown by a dashed line. Only the major orientation of the disordered propyl group is shown.

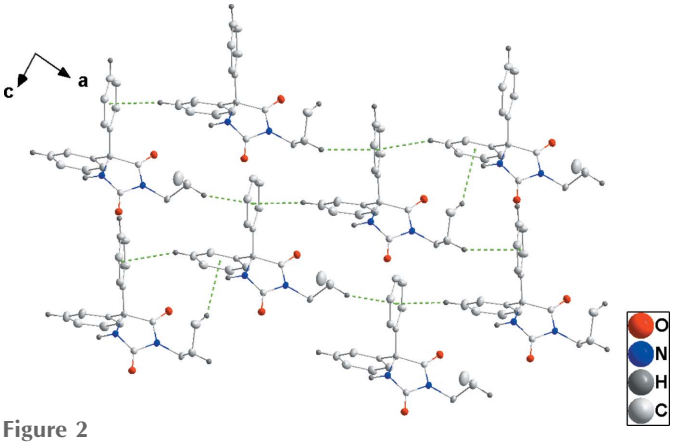


Figure 2
Portion of one layer formed by C—H···π(ring) interactions (green dashed lines) viewed along the *b*-axis direction.

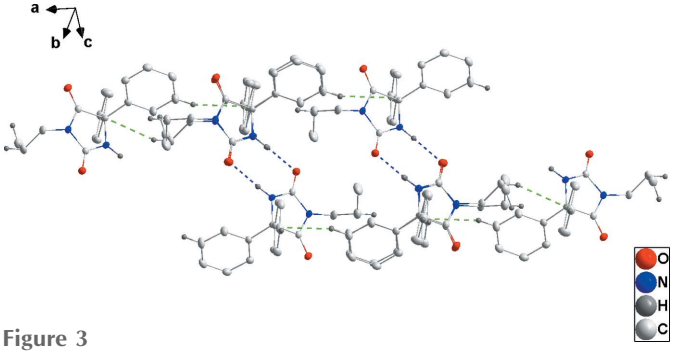


Figure 3
Edge view of two layers showing the inversion-related N—H···O hydrogen bonds (blue dashed lines) holding them together.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{18}N_2O_2$
M_r	294.34
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, *b*, *c* (Å)	9.0951 (5), 13.9582 (7), 14.1083 (7)
α, β, γ (°)	61.646 (1), 80.859 (1), 83.665 (1)
V (Å^3)	1554.92 (14)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	0.08
Crystal size (mm)	0.38 × 0.26 × 0.13
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.90, 0.99
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	30287, 8294, 6452
R_{int}	0.025
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.687
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.050, 0.149, 1.06
No. of reflections	8294
No. of parameters	525
No. of restraints	4
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.82, −0.22

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2016* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

face by inversion-related N2—H2···O4 and N4—H4···O2 hydrogen bonds (Table 1 and Figs. 3 and 4).

Synthesis and crystallization

To a solution of 5,5-diphenylimidazolidine-2,4-dione (3.96 mol, 1 g) in 20 ml of absolute dimethylformamide (DMF) were added equivalent amounts of propyl bromide (3.96 mol), K_2CO_3 (3.96 mol) and a catalytic amount of

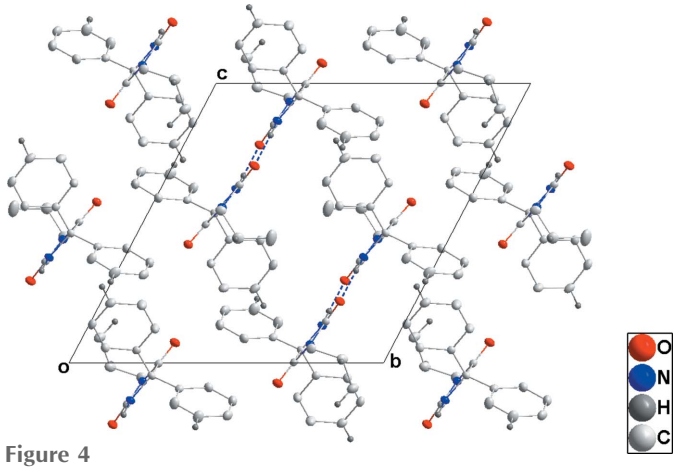


Figure 4
Packing viewed along the *a*-axis direction with intermolecular interactions depicted as in Figs. 2 and 3.

tetrabutylammonium bromide. The resulting solution was heated under reflux for 3 h. The progress was monitored by TLC and, when complete, the solid material was removed by filtration and the solvent evaporated under vacuum. The solid product was purified by recrystallization from an ethanol solution to afford colourless block-like crystals of the title compound (yield 69%).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The *n*-propyl group attached to N3 is disordered over two sites in an 0.859 (2):0.141 (2) ratio. The two components of the disorder were refined subject to restraints that their geometries be comparable.

Acknowledgements

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References

Akrad, R., Mague, J. T., Guerrab, W., Taoufik, J., Ansar, M. & Ramli, Y. (2017). *IUCrData*, **2**, x170033.
Brandenburg, K. & Putz, H. (2012). *DIAMOND*, Crystal Impact GbR, Bonn, Germany.
Bruker (2016). *APEX3*, *SADABS* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Guerrab, W., Akrad, R., Ansar, M., Taoufik, J., Mague, J. T. & Ramli, Y. (2017*a*). *IUCrData*, **2**, x171534.
Guerrab, W., Akrad, R., Ansar, M., Taoufik, J., Mague, J. T. & Ramli, Y. (2017*b*). *IUCrData*, **2**, x171591.
Guerrab, W., Akrad, R., Ansar, M., Taoufik, J., Mague, J. T. & Ramli, Y. (2017*c*). *IUCrData*, **2**, x171693.
Ramli, Y., Akrad, R., Guerrab, W., Taoufik, J., Ansar, M. & Mague, J. T. (2017). *IUCrData*, **2**, x170098.
Ramli, Y., Guerrab, W., Moussaif, A., Taoufik, J., Essassi, E. M. & Mague, J. T. (2017). *IUCrData*, **2**, x171041.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

full crystallographic data

IUCrData (2017). **2**, x171808 [https://doi.org/10.1107/S2414314617018089]

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Crystal data

$C_{18}H_{18}N_2O_2$
M_r = 294.34
Triclinic, $P\overline{1}$
a = 9.0951 (5) Å
b = 13.9582 (7) Å
c = 14.1083 (7) Å
α = 61.646 (1)°
β = 80.859 (1)°
γ = 83.665 (1)°
V = 1554.92 (14) Å^3
Z = 4
$F(000)$ = 624
D_x = 1.257 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9889 reflections
θ = 2.6–29.2°
μ = 0.08 mm^{-1}
T = 100 K
Block, colourless
0.38 × 0.26 × 0.13 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.90, T_{max} = 0.99
30287 measured reflections
8294 independent reflections
6452 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 29.3°, θ_{min} = 1.7°
h = −12→12
k = −19→19
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.149
S = 1.06
8294 reflections
525 parameters
4 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1024P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.82 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Special details

Experimental. The diffraction data were obtained from 3 sets of 400 frames, each of width 0.5° in ω, colllected at φ = 0.00, 90.00 and 180.00° and 2 sets of 800 frames, each of width 0.45° in φ, collected at ω = –30.00 and 210.00°. The scan time was 15 sec/frame.

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger. The *n*-propyl group attached to N3 is disordered over two sites in an 86/14 ratio. The two components of the disorder were refined subject to restraints that their geometries be comparable. The H-atoms attached to the disordered carbon atoms were included as riding contributions in idealized positions.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.48473 (8)	0.18081 (6)	0.42407 (6)	0.01755 (17)	
O2	0.45883 (8)	0.25978 (6)	0.70572 (6)	0.01828 (17)	
N1	0.51038 (9)	0.22639 (7)	0.55718 (6)	0.01434 (18)	
N2	0.27463 (9)	0.24006 (7)	0.62162 (7)	0.01436 (18)	
H2	0.1962 (15)	0.2418 (11)	0.6695 (11)	0.030 (4)*	
C1	0.26504 (10)	0.21140 (8)	0.53557 (7)	0.01268 (19)	
C2	0.43165 (10)	0.20303 (7)	0.49574 (7)	0.01296 (19)	
C3	0.41530 (10)	0.24442 (8)	0.63624 (7)	0.0136 (2)	
C4	0.67315 (11)	0.22770 (9)	0.54519 (8)	0.0184 (2)	
H4A	0.6980 (13)	0.2227 (9)	0.6117 (10)	0.022 (3)*	
H4B	0.7149 (14)	0.1610 (11)	0.5386 (11)	0.035 (4)*	
C5	0.73420 (13)	0.32872 (10)	0.44664 (10)	0.0253 (2)	
H5A	0.8489 (16)	0.3225 (11)	0.4434 (11)	0.043 (4)*	
H5B	0.7070 (14)	0.3307 (11)	0.3781 (11)	0.038 (4)*	
C6	0.67328 (17)	0.43396 (11)	0.44735 (14)	0.0404 (4)	
H6A	0.6946 (18)	0.4252 (13)	0.5188 (15)	0.062 (5)*	
H6B	0.5670 (18)	0.4420 (12)	0.4491 (13)	0.054 (5)*	
H6C	0.7232 (16)	0.4947 (12)	0.3881 (12)	0.043 (4)*	
C7	0.19013 (10)	0.30287 (8)	0.44141 (8)	0.0135 (2)	
C8	0.14852 (11)	0.40325 (8)	0.43836 (8)	0.0166 (2)	
H8	0.1644 (14)	0.4151 (10)	0.4995 (11)	0.029 (3)*	
C9	0.08176 (12)	0.48500 (9)	0.35073 (9)	0.0205 (2)	
H9	0.0494 (16)	0.5548 (12)	0.3491 (12)	0.035 (4)*	
C10	0.05632 (12)	0.46633 (9)	0.26692 (9)	0.0215 (2)	
H10	0.0069 (16)	0.5229 (12)	0.2043 (12)	0.039 (4)*	
C11	0.09900 (12)	0.36686 (9)	0.26855 (9)	0.0209 (2)	
H11	0.0797 (14)	0.3537 (10)	0.2093 (10)	0.026 (3)*	
C12	0.16525 (12)	0.28500 (8)	0.35581 (8)	0.0176 (2)	
H12	0.1954 (13)	0.2153 (10)	0.3587 (10)	0.018 (3)*	
C13	0.18734 (11)	0.10368 (8)	0.58305 (7)	0.0139 (2)	
C14	0.03790 (11)	0.10227 (9)	0.62591 (9)	0.0202 (2)	
H14	−0.0109 (15)	0.1712 (11)	0.6215 (11)	0.034 (4)*	
C15	−0.03798 (12)	0.00581 (9)	0.67654 (9)	0.0240 (2)	
H15	−0.1409 (16)	0.0034 (11)	0.7089 (11)	0.031 (4)*	

C16	0.03532 (13)	−0.09000 (9)	0.68403 (9)	0.0221 (2)	
H16	−0.0178 (15)	−0.1563 (12)	0.7178 (12)	0.034 (4)*	
C17	0.18299 (13)	−0.08871 (9)	0.64096 (9)	0.0219 (2)	
H17	0.2396 (15)	−0.1577 (11)	0.6466 (11)	0.030 (3)*	
C18	0.25930 (12)	0.00795 (8)	0.59043 (8)	0.0182 (2)	
H18	0.3658 (15)	0.0081 (10)	0.5595 (11)	0.027 (3)*	
O3	0.98340 (8)	0.69719 (6)	−0.07289 (6)	0.01940 (17)	
O4	0.95664 (8)	0.75840 (6)	0.22003 (6)	0.01725 (16)	
N3	1.00840 (9)	0.73558 (7)	0.06558 (7)	0.01438 (18)	
N4	0.77230 (9)	0.74262 (7)	0.13330 (7)	0.01473 (18)	
H4	0.6963 (15)	0.7401 (11)	0.1851 (11)	0.027 (3)*	
C19	0.76381 (10)	0.71632 (8)	0.04547 (8)	0.0134 (2)	
C20	0.93049 (10)	0.71417 (8)	0.00219 (8)	0.0136 (2)	
C21	0.91302 (10)	0.74716 (8)	0.14800 (8)	0.0136 (2)	
C22	1.16981 (12)	0.74643 (12)	0.0510 (2)	0.0171 (3)	0.859 (2)
H22A	1.216539	0.722837	−0.003220	0.021*	0.859 (2)
H22B	1.209179	0.697180	0.120576	0.021*	0.859 (2)
C23	1.21427 (13)	0.86212 (10)	0.01399 (10)	0.0210 (3)	0.859 (2)
H23A	1.324353	0.863875	0.003923	0.025*	0.859 (2)
H23B	1.175893	0.883194	0.071471	0.025*	0.859 (2)
C24	1.15523 (17)	0.94499 (11)	−0.09161 (12)	0.0256 (3)	0.859 (2)
H24A	1.192315	1.016896	−0.114047	0.038*	0.859 (2)
H24B	1.046030	0.948307	−0.080446	0.038*	0.859 (2)
H24C	1.189397	0.923007	−0.148175	0.038*	0.859 (2)
C22A	1.1716 (3)	0.7308 (8)	0.0548 (13)	0.0171 (3)	0.141 (2)
H22C	1.211658	0.663810	0.050794	0.021*	0.141 (2)
H22D	1.206032	0.730286	0.118258	0.021*	0.141 (2)
C23A	1.2253 (8)	0.8313 (6)	−0.0489 (6)	0.0210 (3)	0.141 (2)
H23C	1.200510	0.826008	−0.112018	0.025*	0.141 (2)
H23D	1.335132	0.832919	−0.055280	0.025*	0.141 (2)
C24A	1.1560 (12)	0.9370 (6)	−0.0519 (8)	0.0256 (3)	0.141 (2)
H24D	1.165086	0.936914	0.016478	0.038*	0.141 (2)
H24E	1.050473	0.943153	−0.061593	0.038*	0.141 (2)
H24F	1.207935	0.998951	−0.112386	0.038*	0.141 (2)
C25	0.68216 (10)	0.80642 (8)	−0.04580 (8)	0.0140 (2)	
C26	0.65579 (11)	0.91012 (8)	−0.05456 (8)	0.0173 (2)	
H26	0.6869 (14)	0.9260 (10)	0.0004 (11)	0.029 (3)*	
C27	0.58340 (12)	0.99113 (9)	−0.13937 (9)	0.0197 (2)	
H27	0.5658 (16)	1.0636 (12)	−0.1460 (12)	0.040 (4)*	
C28	0.53733 (12)	0.96829 (9)	−0.21508 (9)	0.0210 (2)	
H28	0.4791 (16)	1.0221 (12)	−0.2728 (12)	0.042 (4)*	
C29	0.56533 (13)	0.86544 (9)	−0.20771 (9)	0.0249 (2)	
H29	0.5340 (15)	0.8493 (11)	−0.2617 (12)	0.038 (4)*	
C30	0.63728 (13)	0.78448 (9)	−0.12344 (9)	0.0219 (2)	
H30	0.6600 (15)	0.7118 (12)	−0.1186 (11)	0.032 (4)*	
C31	0.69286 (11)	0.60606 (8)	0.09187 (8)	0.0144 (2)	
C32	0.76638 (12)	0.51533 (8)	0.08758 (9)	0.0187 (2)	
H32	0.8703 (15)	0.5229 (11)	0.0483 (11)	0.027 (3)*	

C33	0.69545 (13)	0.41643 (9)	0.13573 (9)	0.0226 (2)
H33	0.7532 (15)	0.3508 (11)	0.1336 (11)	0.033 (4)*
C34	0.55150 (13)	0.40801 (9)	0.18795 (9)	0.0228 (2)
H34	0.5058 (16)	0.3381 (12)	0.2211 (12)	0.037 (4)*
C35	0.47705 (13)	0.49878 (9)	0.19224 (10)	0.0253 (2)
H35	0.3752 (16)	0.4911 (11)	0.2297 (11)	0.033 (4)*
C36	0.54751 (12)	0.59709 (9)	0.14439 (9)	0.0223 (2)
H36	0.4963 (15)	0.6607 (12)	0.1505 (11)	0.036 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0169 (4)	0.0205 (4)	0.0159 (3)	−0.0007 (3)	0.0003 (3)	−0.0098 (3)
O2	0.0158 (4)	0.0255 (4)	0.0171 (4)	−0.0018 (3)	−0.0029 (3)	−0.0124 (3)
N1	0.0100 (4)	0.0184 (4)	0.0143 (4)	−0.0007 (3)	−0.0003 (3)	−0.0077 (3)
N2	0.0120 (4)	0.0197 (4)	0.0139 (4)	−0.0010 (3)	−0.0008 (3)	−0.0101 (3)
C1	0.0111 (4)	0.0145 (5)	0.0136 (4)	−0.0002 (3)	−0.0009 (3)	−0.0078 (4)
C2	0.0127 (4)	0.0108 (4)	0.0122 (4)	−0.0001 (3)	−0.0017 (3)	−0.0028 (4)
C3	0.0125 (5)	0.0134 (5)	0.0126 (4)	−0.0013 (3)	−0.0002 (3)	−0.0044 (4)
C4	0.0098 (5)	0.0252 (5)	0.0191 (5)	−0.0001 (4)	−0.0017 (4)	−0.0096 (4)
C5	0.0192 (5)	0.0286 (6)	0.0268 (6)	−0.0057 (4)	0.0009 (4)	−0.0119 (5)
C6	0.0348 (8)	0.0251 (7)	0.0589 (10)	−0.0108 (6)	0.0067 (7)	−0.0194 (7)
C7	0.0114 (4)	0.0136 (5)	0.0141 (4)	−0.0018 (3)	−0.0014 (3)	−0.0051 (4)
C8	0.0154 (5)	0.0156 (5)	0.0192 (5)	−0.0010 (4)	−0.0014 (4)	−0.0086 (4)
C9	0.0192 (5)	0.0142 (5)	0.0243 (5)	0.0007 (4)	−0.0029 (4)	−0.0061 (4)
C10	0.0200 (5)	0.0164 (5)	0.0207 (5)	−0.0017 (4)	−0.0061 (4)	−0.0015 (4)
C11	0.0240 (5)	0.0197 (5)	0.0172 (5)	−0.0022 (4)	−0.0071 (4)	−0.0057 (4)
C12	0.0211 (5)	0.0154 (5)	0.0169 (5)	−0.0003 (4)	−0.0046 (4)	−0.0075 (4)
C13	0.0145 (5)	0.0143 (5)	0.0118 (4)	−0.0019 (4)	−0.0023 (3)	−0.0046 (4)
C14	0.0145 (5)	0.0169 (5)	0.0251 (5)	−0.0003 (4)	−0.0017 (4)	−0.0067 (4)
C15	0.0154 (5)	0.0231 (6)	0.0269 (6)	−0.0049 (4)	−0.0008 (4)	−0.0059 (5)
C16	0.0261 (6)	0.0176 (5)	0.0198 (5)	−0.0084 (4)	−0.0029 (4)	−0.0050 (4)
C17	0.0285 (6)	0.0162 (5)	0.0214 (5)	−0.0013 (4)	−0.0015 (4)	−0.0096 (4)
C18	0.0185 (5)	0.0174 (5)	0.0188 (5)	−0.0013 (4)	0.0001 (4)	−0.0091 (4)
O3	0.0186 (4)	0.0245 (4)	0.0165 (4)	−0.0013 (3)	0.0006 (3)	−0.0114 (3)
O4	0.0155 (4)	0.0224 (4)	0.0164 (3)	−0.0007 (3)	−0.0031 (3)	−0.0109 (3)
N3	0.0109 (4)	0.0173 (4)	0.0151 (4)	−0.0003 (3)	−0.0006 (3)	−0.0080 (3)
N4	0.0122 (4)	0.0201 (4)	0.0139 (4)	−0.0009 (3)	−0.0008 (3)	−0.0097 (3)
C19	0.0126 (4)	0.0158 (5)	0.0135 (4)	−0.0002 (4)	−0.0012 (3)	−0.0083 (4)
C20	0.0131 (5)	0.0119 (4)	0.0135 (4)	−0.0006 (3)	−0.0016 (3)	−0.0039 (4)
C21	0.0136 (5)	0.0119 (4)	0.0136 (4)	−0.0008 (3)	−0.0009 (3)	−0.0048 (4)
C22	0.0098 (5)	0.0200 (7)	0.0204 (5)	−0.0006 (4)	−0.0007 (4)	−0.0088 (6)
C23	0.0176 (6)	0.0264 (7)	0.0203 (6)	−0.0082 (5)	−0.0008 (4)	−0.0109 (5)
C24	0.0283 (7)	0.0226 (6)	0.0214 (8)	−0.0070 (5)	−0.0042 (7)	−0.0051 (6)
C22A	0.0098 (5)	0.0200 (7)	0.0204 (5)	−0.0006 (4)	−0.0007 (4)	−0.0088 (6)
C23A	0.0176 (6)	0.0264 (7)	0.0203 (6)	−0.0082 (5)	−0.0008 (4)	−0.0109 (5)
C24A	0.0283 (7)	0.0226 (6)	0.0214 (8)	−0.0070 (5)	−0.0042 (7)	−0.0051 (6)
C25	0.0121 (4)	0.0144 (5)	0.0142 (4)	−0.0010 (4)	−0.0011 (3)	−0.0057 (4)

C26	0.0174 (5)	0.0170 (5)	0.0190 (5)	−0.0015 (4)	−0.0023 (4)	−0.0093 (4)
C27	0.0201 (5)	0.0137 (5)	0.0229 (5)	0.0003 (4)	−0.0021 (4)	−0.0069 (4)
C28	0.0201 (5)	0.0186 (5)	0.0192 (5)	0.0000 (4)	−0.0052 (4)	−0.0041 (4)
C29	0.0338 (6)	0.0210 (5)	0.0223 (5)	0.0021 (5)	−0.0128 (5)	−0.0097 (5)
C30	0.0295 (6)	0.0180 (5)	0.0213 (5)	0.0024 (4)	−0.0103 (4)	−0.0101 (4)
C31	0.0144 (5)	0.0146 (5)	0.0135 (4)	−0.0012 (4)	−0.0033 (3)	−0.0054 (4)
C32	0.0188 (5)	0.0190 (5)	0.0196 (5)	0.0003 (4)	−0.0010 (4)	−0.0105 (4)
C33	0.0283 (6)	0.0171 (5)	0.0237 (5)	−0.0001 (4)	−0.0031 (4)	−0.0107 (4)
C34	0.0275 (6)	0.0175 (5)	0.0215 (5)	−0.0071 (4)	−0.0025 (4)	−0.0063 (4)
C35	0.0188 (5)	0.0232 (6)	0.0311 (6)	−0.0058 (4)	0.0022 (4)	−0.0109 (5)
C36	0.0148 (5)	0.0208 (5)	0.0313 (6)	−0.0012 (4)	0.0003 (4)	−0.0129 (5)

Geometric parameters (Å, º)

O1—C2	1.2090 (11)	N3—C22A	1.466 (3)
O2—C3	1.2269 (11)	N4—C21	1.3416 (12)
N1—C2	1.3739 (12)	N4—C19	1.4646 (11)
N1—C3	1.4026 (12)	N4—H4	0.913 (14)
N1—C4	1.4642 (12)	C19—C31	1.5302 (13)
N2—C3	1.3402 (12)	C19—C25	1.5332 (13)
N2—C1	1.4643 (11)	C19—C20	1.5444 (13)
N2—H2	0.908 (14)	C22—C23	1.523 (2)
C1—C13	1.5285 (13)	C22—H22A	0.9900
C1—C7	1.5310 (13)	C22—H22B	0.9900
C1—C2	1.5421 (13)	C23—C24	1.5251 (18)
C4—C5	1.5149 (15)	C23—H23A	0.9900
C4—H4A	0.969 (12)	C23—H23B	0.9900
C4—H4B	1.006 (13)	C24—H24A	0.9800
C5—C6	1.5156 (18)	C24—H24B	0.9800
C5—H5A	1.033 (14)	C24—H24C	0.9800
C5—H5B	1.022 (14)	C22A—C23A	1.523 (4)
C6—H6A	1.004 (17)	C22A—H22C	0.9900
C6—H6B	0.958 (16)	C22A—H22D	0.9900
C6—H6C	0.957 (15)	C23A—C24A	1.523 (3)
C7—C8	1.3925 (13)	C23A—H23C	0.9900
C7—C12	1.3991 (13)	C23A—H23D	0.9900
C8—C9	1.3946 (14)	C24A—H24D	0.9800
C8—H8	0.985 (13)	C24A—H24E	0.9800
C9—C10	1.3830 (15)	C24A—H24F	0.9800
C9—H9	0.977 (15)	C25—C26	1.3896 (13)
C10—C11	1.3901 (15)	C25—C30	1.3959 (13)
C10—H10	0.996 (15)	C26—C27	1.3946 (14)
C11—C12	1.3899 (14)	C26—H26	0.989 (13)
C11—H11	0.981 (13)	C27—C28	1.3832 (15)
C12—H12	0.965 (12)	C27—H27	0.968 (15)
C13—C18	1.3861 (13)	C28—C29	1.3865 (15)
C13—C14	1.3952 (14)	C28—H28	0.988 (15)
C14—C15	1.3908 (14)	C29—C30	1.3880 (15)

C14—H14	0.992 (14)	C29—H29	0.979 (14)
C15—C16	1.3913 (16)	C30—H30	0.985 (14)
C15—H15	0.971 (14)	C31—C32	1.3884 (13)
C16—C17	1.3816 (16)	C31—C36	1.3963 (14)
C16—H16	0.961 (15)	C32—C33	1.3963 (14)
C17—C18	1.3951 (14)	C32—H32	1.006 (13)
C17—H17	1.014 (14)	C33—C34	1.3842 (16)
C18—H18	0.997 (13)	C33—H33	1.015 (14)
O3—C20	1.2087 (11)	C34—C35	1.3921 (15)
O4—C21	1.2279 (11)	C34—H34	0.968 (15)
N3—C20	1.3759 (12)	C35—C36	1.3878 (15)
N3—C21	1.3993 (12)	C35—H35	0.981 (14)
N3—C22	1.4642 (13)	C36—H36	0.990 (14)

C2—N1—C3	111.38 (8)	C31—C19—C25	111.92 (7)
C2—N1—C4	124.52 (8)	N4—C19—C20	100.77 (7)
C3—N1—C4	124.05 (8)	C31—C19—C20	113.17 (8)
C3—N2—C1	113.01 (8)	C25—C19—C20	108.44 (7)
C3—N2—H2	121.6 (8)	O3—C20—N3	126.18 (9)
C1—N2—H2	124.3 (8)	O3—C20—C19	127.03 (8)
N2—C1—C13	109.91 (8)	N3—C20—C19	106.80 (8)
N2—C1—C7	112.14 (8)	O4—C21—N4	128.22 (9)
C13—C1—C7	112.17 (7)	O4—C21—N3	123.68 (9)
N2—C1—C2	100.74 (7)	N4—C21—N3	108.10 (8)
C13—C1—C2	113.12 (7)	N3—C22—C23	113.35 (11)
C7—C1—C2	108.24 (7)	N3—C22—H22A	108.9
O1—C2—N1	125.81 (9)	C23—C22—H22A	108.9
O1—C2—C1	127.32 (8)	N3—C22—H22B	108.9
N1—C2—C1	106.87 (8)	C23—C22—H22B	108.9
O2—C3—N2	128.17 (9)	H22A—C22—H22B	107.7
O2—C3—N1	123.97 (9)	C22—C23—C24	112.92 (14)
N2—C3—N1	107.85 (8)	C22—C23—H23A	109.0
N1—C4—C5	112.45 (9)	C24—C23—H23A	109.0
N1—C4—H4A	106.0 (7)	C22—C23—H23B	109.0
C5—C4—H4A	111.6 (7)	C24—C23—H23B	109.0
N1—C4—H4B	107.8 (7)	H23A—C23—H23B	107.8
C5—C4—H4B	109.5 (8)	C23—C24—H24A	109.5
H4A—C4—H4B	109.3 (10)	C23—C24—H24B	109.5
C4—C5—C6	113.45 (10)	H24A—C24—H24B	109.5
C4—C5—H5A	107.5 (8)	C23—C24—H24C	109.5
C6—C5—H5A	110.9 (7)	H24A—C24—H24C	109.5
C4—C5—H5B	109.3 (7)	H24B—C24—H24C	109.5
C6—C5—H5B	107.4 (7)	N3—C22A—C23A	107.4 (5)
H5A—C5—H5B	108.2 (10)	N3—C22A—H22C	110.2
C5—C6—H6A	104.3 (10)	C23A—C22A—H22C	110.2
C5—C6—H6B	112.3 (9)	N3—C22A—H22D	110.2
H6A—C6—H6B	105.8 (13)	C23A—C22A—H22D	110.2
C5—C6—H6C	110.3 (9)	H22C—C22A—H22D	108.5

H6A—C6—H6C	111.0 (12)	C22A—C23A—C24A	112.7 (5)
H6B—C6—H6C	112.7 (13)	C22A—C23A—H23C	109.1
C8—C7—C12	119.55 (9)	C24A—C23A—H23C	109.1
C8—C7—C1	121.69 (8)	C22A—C23A—H23D	109.1
C12—C7—C1	118.75 (8)	C24A—C23A—H23D	109.1
C7—C8—C9	120.06 (9)	H23C—C23A—H23D	107.8
C7—C8—H8	119.3 (8)	C23A—C24A—H24D	109.5
C9—C8—H8	120.6 (8)	C23A—C24A—H24E	109.5
C10—C9—C8	120.03 (10)	H24C—C24A—H24D	109.5
C10—C9—H9	119.4 (8)	C23A—C24A—H24F	109.5
C8—C9—H9	120.5 (9)	H24D—C24A—H24F	109.5
C9—C10—C11	120.37 (10)	H24E—C24A—H24F	109.5
C9—C10—H10	121.5 (8)	C26—C25—C30	119.40 (9)
C11—C10—H10	118.2 (8)	C26—C25—C19	121.42 (8)
C12—C11—C10	119.84 (10)	C30—C25—C19	119.16 (8)
C12—C11—H11	120.1 (8)	C25—C26—C27	120.28 (9)
C10—C11—H11	120.1 (8)	C25—C26—H26	119.8 (8)
C11—C12—C7	120.14 (9)	C27—C26—H26	119.9 (8)
C11—C12—H12	121.2 (7)	C28—C27—C26	119.96 (9)
C7—C12—H12	118.7 (7)	C28—C27—H27	119.6 (9)
C18—C13—C14	119.27 (9)	C26—C27—H27	120.4 (9)
C18—C13—C1	123.53 (9)	C27—C28—C29	120.02 (10)
C14—C13—C1	117.11 (8)	C27—C28—H28	121.9 (8)
C15—C14—C13	120.54 (10)	C29—C28—H28	118.0 (8)
C15—C14—H14	121.4 (8)	C28—C29—C30	120.26 (10)
C13—C14—H14	118.1 (8)	C28—C29—H29	120.2 (8)
C14—C15—C16	119.80 (10)	C30—C29—H29	119.5 (8)
C14—C15—H15	121.2 (8)	C29—C30—C25	120.06 (10)
C16—C15—H15	119.0 (8)	C29—C30—H30	120.8 (8)
C17—C16—C15	119.80 (10)	C25—C30—H30	119.1 (8)
C17—C16—H16	120.5 (8)	C32—C31—C36	119.19 (9)
C15—C16—H16	119.7 (8)	C32—C31—C19	123.76 (9)
C16—C17—C18	120.43 (10)	C36—C31—C19	117.01 (9)
C16—C17—H17	121.4 (8)	C31—C32—C33	120.14 (10)
C18—C17—H17	118.2 (8)	C31—C32—H32	118.7 (7)
C13—C18—C17	120.15 (10)	C33—C32—H32	121.2 (7)
C13—C18—H18	120.0 (7)	C34—C33—C32	120.38 (10)
C17—C18—H18	119.9 (7)	C34—C33—H33	121.2 (8)
C20—N3—C21	111.29 (8)	C32—C33—H33	118.4 (8)
C20—N3—C22	125.95 (15)	C33—C34—C35	119.74 (10)
C21—N3—C22	122.75 (15)	C33—C34—H34	118.4 (8)
C20—N3—C22A	122.5 (9)	C35—C34—H34	121.9 (8)
C21—N3—C22A	125.6 (9)	C36—C35—C34	119.89 (10)
C21—N4—C19	112.74 (8)	C36—C35—H35	121.6 (8)
C21—N4—H4	119.3 (8)	C34—C35—H35	118.5 (8)
C19—N4—H4	126.3 (8)	C35—C36—C31	120.65 (10)
N4—C19—C31	109.65 (8)	C35—C36—H36	119.9 (8)
N4—C19—C25	112.43 (8)	C31—C36—H36	119.4 (8)

C3—N2—C1—C13	117.44 (9)	C22—N3—C20—O3	2.79 (16)
C3—N2—C1—C7	−117.06 (9)	C22A—N3—C20—O3	−5.6 (3)
C3—N2—C1—C2	−2.15 (10)	C21—N3—C20—C19	2.39 (10)
C3—N1—C2—O1	−177.65 (9)	C22—N3—C20—C19	−177.12 (9)
C4—N1—C2—O1	−0.14 (15)	C22A—N3—C20—C19	174.5 (3)
C3—N1—C2—C1	2.65 (10)	N4—C19—C20—O3	−178.94 (9)
C4—N1—C2—C1	−179.84 (8)	C31—C19—C20—O3	64.08 (12)
N2—C1—C2—O1	179.94 (9)	C25—C19—C20—O3	−60.72 (12)
C13—C1—C2—O1	62.69 (12)	N4—C19—C20—N3	0.97 (9)
C7—C1—C2—O1	−62.26 (12)	C31—C19—C20—N3	−116.02 (8)
N2—C1—C2—N1	−0.37 (9)	C25—C19—C20—N3	119.18 (8)
C13—C1—C2—N1	−117.62 (8)	C19—N4—C21—O4	−173.52 (9)
C7—C1—C2—N1	117.43 (8)	C19—N4—C21—N3	5.89 (11)
C1—N2—C3—O2	−175.31 (9)	C20—N3—C21—O4	174.30 (9)
C1—N2—C3—N1	3.84 (11)	C22—N3—C21—O4	−6.17 (15)
C2—N1—C3—O2	175.12 (9)	C22A—N3—C21—O4	2.5 (4)
C4—N1—C3—O2	−2.40 (15)	C20—N3—C21—N4	−5.14 (11)
C2—N1—C3—N2	−4.07 (11)	C22—N3—C21—N4	174.39 (9)
C4—N1—C3—N2	178.41 (9)	C22A—N3—C21—N4	−176.9 (4)
C2—N1—C4—C5	76.00 (12)	C20—N3—C22—C23	111.2 (2)
C3—N1—C4—C5	−106.80 (11)	C21—N3—C22—C23	−68.2 (2)
N1—C4—C5—C6	58.11 (14)	N3—C22—C23—C24	−57.2 (2)
N2—C1—C7—C8	4.56 (12)	C20—N3—C22A—C23A	74.1 (12)
C13—C1—C7—C8	128.82 (9)	C21—N3—C22A—C23A	−115.0 (10)
C2—C1—C7—C8	−105.67 (10)	N3—C22A—C23A—C24A	54.6 (15)
N2—C1—C7—C12	−176.39 (8)	N4—C19—C25—C26	15.27 (12)
C13—C1—C7—C12	−52.13 (11)	C31—C19—C25—C26	139.20 (9)
C2—C1—C7—C12	73.38 (10)	C20—C19—C25—C26	−95.26 (10)
C12—C7—C8—C9	0.36 (15)	N4—C19—C25—C30	−166.60 (9)
C1—C7—C8—C9	179.40 (9)	C31—C19—C25—C30	−42.67 (12)
C7—C8—C9—C10	0.23 (15)	C20—C19—C25—C30	82.87 (11)
C8—C9—C10—C11	−0.98 (16)	C30—C25—C26—C27	0.84 (15)
C9—C10—C11—C12	1.14 (16)	C19—C25—C26—C27	178.96 (9)
C10—C11—C12—C7	−0.54 (16)	C25—C26—C27—C28	0.11 (16)
C8—C7—C12—C11	−0.20 (15)	C26—C27—C28—C29	−1.08 (16)
C1—C7—C12—C11	−179.27 (9)	C27—C28—C29—C30	1.12 (17)
N2—C1—C13—C18	−111.24 (10)	C28—C29—C30—C25	−0.17 (17)
C7—C1—C13—C18	123.27 (10)	C26—C25—C30—C29	−0.80 (16)
C2—C1—C13—C18	0.48 (13)	C19—C25—C30—C29	−178.97 (10)
N2—C1—C13—C14	65.31 (11)	N4—C19—C31—C32	−116.77 (10)
C7—C1—C13—C14	−60.18 (11)	C25—C19—C31—C32	117.75 (10)
C2—C1—C13—C14	177.03 (8)	C20—C19—C31—C32	−5.14 (13)
C18—C13—C14—C15	0.66 (15)	N4—C19—C31—C36	60.99 (11)
C1—C13—C14—C15	−176.04 (9)	C25—C19—C31—C36	−64.49 (11)
C13—C14—C15—C16	−0.36 (17)	C20—C19—C31—C36	172.62 (9)
C14—C15—C16—C17	−0.11 (16)	C36—C31—C32—C33	−0.25 (15)
C15—C16—C17—C18	0.29 (16)	C19—C31—C32—C33	177.46 (9)

C14—C13—C18—C17	−0.48 (15)	C31—C32—C33—C34	0.06 (16)
C1—C13—C18—C17	176.00 (9)	C32—C33—C34—C35	0.13 (16)
C16—C17—C18—C13	0.01 (16)	C33—C34—C35—C36	−0.13 (17)
C21—N4—C19—C31	115.33 (9)	C34—C35—C36—C31	−0.07 (17)
C21—N4—C19—C25	−119.49 (9)	C32—C31—C36—C35	0.26 (16)
C21—N4—C19—C20	−4.22 (10)	C19—C31—C36—C35	−177.61 (10)
C21—N3—C20—O3	−177.70 (9)		

Hydrogen-bond geometry (Å, º)

Cg2, Cg5 and Cg6 are the centroids of the C25–C30, C7–C12 and C13–C18 phenyl rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O4^{i}	0.908 (14)	1.915 (15)	2.8211 (11)	174.8 (12)
N4—H4···O2^{i}	0.913 (14)	1.917 (14)	2.8293 (10)	177.3 (12)
C5—H5*A*···*Cg*5^{ii}	1.033 (15)	2.651 (15)	3.6101 (13)	154.4 (11)
C15—H15···*Cg*2^{iii}	0.971 (15)	2.925 (14)	3.8055 (12)	154.1 (12)
C23—H23*A*···*Cg*2^{ii}	0.99	2.92	3.8118 (15)	151
C24—H24*C*···*Cg*6^{iv}	0.98	2.91	3.6320 (13)	131
C35—H35···*Cg*5	0.981 (15)	2.741 (15)	3.6627 (13)	156.9 (13)

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