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3-Benzyl-5,5-diphenylimidazolidine-2,4-dione

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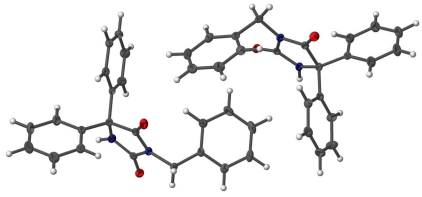
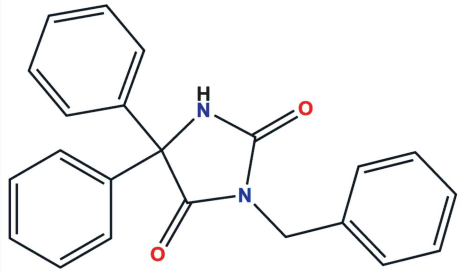
The asymmetric unit of the title compound, $C_{22}H_{18}N_2O_2$, consists of two independent molecules differing primarily in the orientation of the benzyl substituent. The two independent molecules are associated through complementary C—H···π interactions and are elaborated into corrugated sheets by paired N—H···O and C—H···O hydrogen bonds. Additional C—H···O hydrogen bonds bind the sheets together.

3D view



Chemical scheme



Structure description

As a continuation of our studies of phenytoin derivatives (Ramli, Akrad *et al.*, 2017; Ramli, Guerrab *et al.*, 2017; Akrad *et al.*, 2017; Guerrab *et al.*, 2017*a*,*b*,*c*), we report herein the synthesis and crystal structure of the new title 5,5-diphenylimidazolidine derivative.

The asymmetric unit of the title compound consists of two independent molecules which differ in the orientations of the benzyl groups (Fig. 1). Thus the N1—C4—C5—C6 torsion angle is 26.89 (15)°, while the N3—C26—C27—C28 torsion angle is 70.96 (13)°. Each imidazolidine-2,4-dione ring has two phenyl groups attached to the 5-position. The C11–C16 and C17–C22 phenyl rings are inclined to the C1/C2/N1/C3/N2 ring by 71.62 (6) and 72.22 (7)°, respectively, while the C33–C38 and C39–C44 phenyl rings are inclined to the C23/C24/N3/C25/N4 ring by 70.22 (6) and 77.25 (7)°, respectively.

In the crystal, the two independent molecules are associated through C—H···π interactions (C8—H8···*Cg*7 and C31—H31···*Cg*3; Table 1 and Fig. 1; *Cg*3 and *Cg*7 are the centroids of the C11–C16 and C33–C38 phenyl rings, respectively) and are coupled to a second such unit by inversion-related C15—H15···O3 hydrogen bonds and offset π–π stacking interactions between C27–C32 phenyl rings [Table 1 and Fig. 2; centroid–centroid distance = 3.9033 (8) Å. Inversion-related N2—H2···O2 and N4—H4···O4 hydrogen bonds bind this tetramolecular unit to two further similar units to ultimately

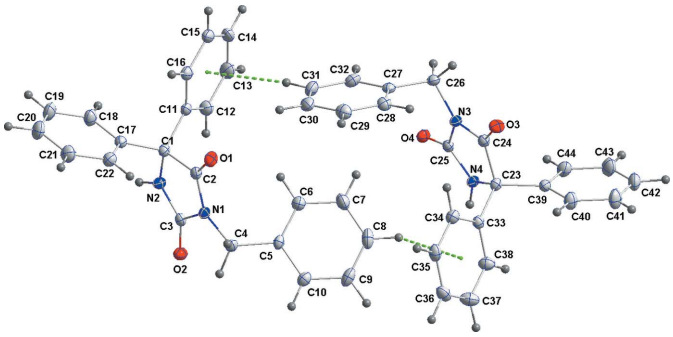


Figure 1
The asymmetric unit with labeling scheme and 50% probability displacement ellipsoids. The C—H···π(ring) interactions are shown by dashed lines.

form a thick, corrugated sheet (Table 1 and Fig. 2). The sheets are linked *via* C15—H15···O3 hydrogen bonds (Table 1 and Figs. 3 and 4).

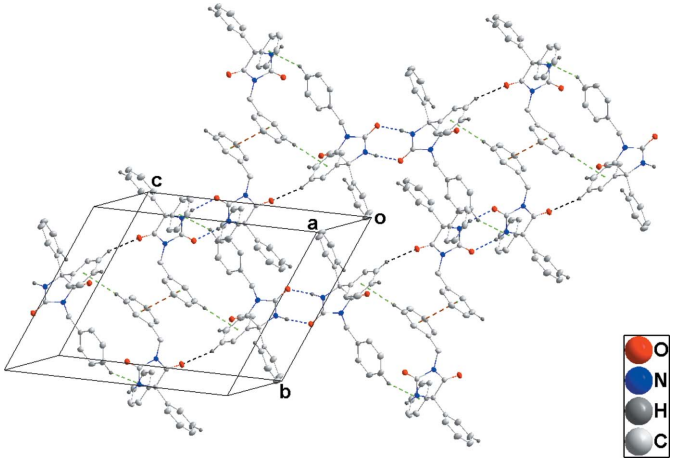


Figure 2
Detail of the interactions forming one corrugated sheet. N—H···O and C—H···O hydrogen bonds are shown, respectively, by blue and black dashed lines while C—H···π(ring) and π–π stacking interactions are shown by green and orange dashed lines.

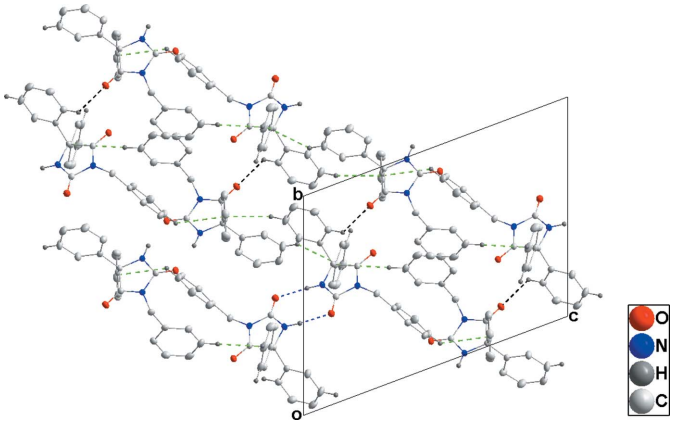


Figure 3
Detail of the C—H···O hydrogen bonding holding the sheets together viewed along the *a*-axis direction. Color codes are the same as in Fig. 2.

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

*Cg*3 and *Cg*7 are the centroids of the C11–C16 and C33–C38 phenyl rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O2^{i}	0.918 (16)	1.930 (16)	2.8446 (13)	173.3 (14)
N4—H4···O4^{ii}	0.916 (15)	1.958 (15)	2.8613 (12)	168.3 (14)
C8—H8···*Cg*7	0.985 (16)	2.987 (16)	3.5734 (14)	119.3 (11)
C15—H15···O3^{iii}	0.978 (15)	2.451 (16)	3.3830 (17)	159.2 (13)
C19—H19···*Cg*7^{iv}	0.983 (17)	2.732 (17)	3.6805 (15)	162.4 (14)
C22—H22···O3^{v}	0.973 (13)	2.586 (14)	3.3111 (15)	131.4 (11)
C31—H31···*Cg*3	0.981 (16)	2.917 (15)	3.8944 (15)	174.2 (12)
C41—H41···*Cg*3^{vi}	0.951 (17)	2.830 (17)	3.6570 (15)	146.0 (15)

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $-x+2, -y, -z+1$; (iii) $-x+2, -y+1, -z+1$; (iv) $x, y+1, z-1$; (v) $-x+1, -y+1, -z+1$; (vi) $x, y-1, z+1$.

Synthesis and crystallization

To a solution of 5,5-diphenylimidazolidine-2,4-dione (3.96 mol, 1 g) in 20 ml of dimethylformamide (DMF) were added one equivalent of benzyl chloride (3.96 mol), K_2CO_3 (3.96 mol) and a catalytic amount of tetrabutylammonium bromide. The solution was heated under reflux for 3 h. The progress was monitored by TLC and after completion the solid material was removed by filtration and the solvent evaporated under vacuum. The solid product was purified by recrystallization from ethanol solution to afford colorless block-like crystals of the title compound (yield 69%).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

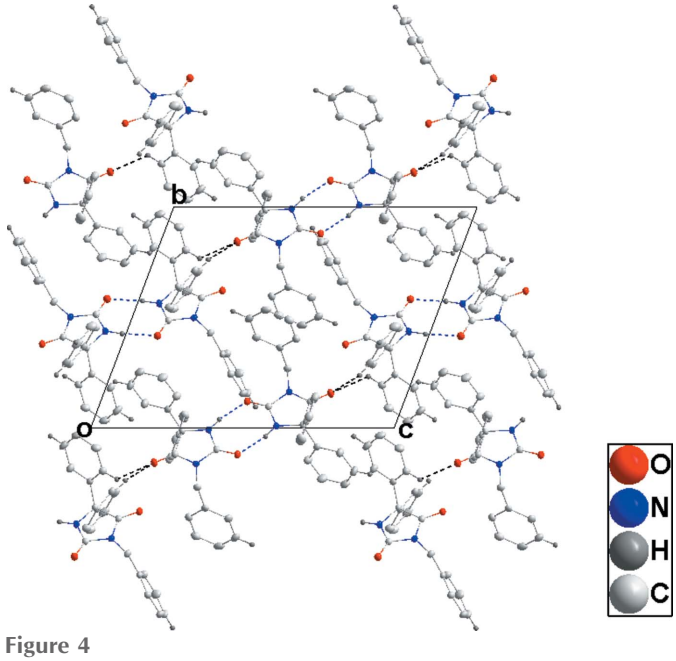


Figure 4
Packing viewed along the *a*-axis direction. Color codes are the same as in Fig. 2.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{22}H_{18}N_2O_2$
M_r	342.38
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, b, c (Å)	8.8897 (5), 13.2911 (7), 16.6864 (9)
α, β, γ (°)	67.900 (1), 81.027 (1), 74.294 (1)
V (Å^3)	1755.27 (17)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.37 × 0.21 × 0.19
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.90, 0.98
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	34377, 9388, 7122
R_{int}	0.035
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.689
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.047, 0.129, 1.03
No. of reflections	9388
No. of parameters	613
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.43, −0.20

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

Acknowledgements

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full crystallographic data

IUCrData (2018). **3**, x171832 [https://doi.org/10.1107/S2414314617018326]

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3-Benzyl-5,5-diphenylimidazolidine-2,4-dione

Crystal data

$C_{22}H_{18}N_2O_2$
M_r = 342.38
Triclinic, $P\overline{1}$
a = 8.8897 (5) Å
b = 13.2911 (7) Å
c = 16.6864 (9) Å
α = 67.900 (1)°
β = 81.027 (1)°
γ = 74.294 (1)°
V = 1755.27 (17) Å^3
Z = 4
$F(000)$ = 720
D_x = 1.296 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9954 reflections
θ = 2.4–29.2°
μ = 0.08 mm^{-1}
T = 100 K
Block, colourless
0.37 × 0.21 × 0.19 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} = 0.98
34377 measured reflections
9388 independent reflections
7122 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 29.3°, θ_{min} = 1.7°
h = −12→12
k = −18→18
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.129
S = 1.03
9388 reflections
613 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0832P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.46307 (9)	0.62158 (7)	0.26376 (5)	0.02014 (18)
O2	0.41552 (9)	0.41700 (7)	0.10586 (5)	0.01982 (18)
N1	0.42911 (10)	0.49893 (7)	0.20433 (6)	0.01533 (19)
N2	0.53687 (11)	0.56296 (8)	0.07157 (6)	0.0166 (2)
H2	0.5562 (16)	0.5738 (12)	0.0136 (10)	0.031 (4)*
C1	0.55306 (12)	0.63913 (9)	0.11229 (7)	0.0145 (2)
C2	0.47733 (12)	0.58910 (9)	0.20364 (7)	0.0149 (2)
C3	0.45820 (12)	0.48636 (9)	0.12306 (7)	0.0149 (2)
C4	0.34479 (13)	0.43039 (9)	0.27741 (7)	0.0171 (2)
H4A	0.2760 (16)	0.4038 (11)	0.2521 (9)	0.023 (3)*
H4B	0.2729 (14)	0.4810 (11)	0.3073 (8)	0.017 (3)*
C5	0.44722 (13)	0.33415 (9)	0.34260 (7)	0.0158 (2)
C6	0.59706 (14)	0.33556 (10)	0.35577 (8)	0.0218 (2)
H6	0.6439 (17)	0.3995 (12)	0.3179 (10)	0.029 (4)*
C7	0.68251 (15)	0.24753 (11)	0.42072 (9)	0.0269 (3)
H7	0.787 (2)	0.2494 (14)	0.4296 (11)	0.049 (5)*
C8	0.61849 (16)	0.15808 (11)	0.47286 (8)	0.0271 (3)
H8	0.6812 (17)	0.0949 (13)	0.5171 (10)	0.037 (4)*
C9	0.46925 (15)	0.15669 (10)	0.46011 (8)	0.0253 (3)
H9	0.4252 (17)	0.0926 (13)	0.4982 (10)	0.036 (4)*
C10	0.38403 (14)	0.24386 (9)	0.39524 (8)	0.0195 (2)
H10	0.2836 (18)	0.2390 (12)	0.3863 (10)	0.031 (4)*
C11	0.72450 (12)	0.63221 (9)	0.12231 (7)	0.0162 (2)
C12	0.84449 (14)	0.54637 (10)	0.11023 (8)	0.0232 (3)
H12	0.8223 (16)	0.4901 (12)	0.0918 (10)	0.030 (4)*
C13	0.99862 (15)	0.54048 (11)	0.12297 (9)	0.0289 (3)
H13	1.0850 (17)	0.4806 (13)	0.1125 (10)	0.034 (4)*
C14	1.03148 (15)	0.61956 (11)	0.14806 (9)	0.0278 (3)
H14	1.1406 (17)	0.6137 (12)	0.1550 (10)	0.032 (4)*
C15	0.91174 (15)	0.70524 (11)	0.16108 (8)	0.0246 (3)
H15	0.9348 (17)	0.7615 (12)	0.1788 (10)	0.031 (4)*
C16	0.75873 (14)	0.71171 (10)	0.14773 (7)	0.0193 (2)
H16	0.6712 (16)	0.7742 (12)	0.1554 (9)	0.025 (4)*
C17	0.46350 (12)	0.75773 (9)	0.06344 (7)	0.0162 (2)
C18	0.52722 (14)	0.81724 (11)	−0.01667 (8)	0.0242 (3)
H18	0.6320 (17)	0.7822 (12)	−0.0394 (9)	0.029 (4)*

C19	0.44513 (16)	0.92154 (11)	−0.06618 (9)	0.0307 (3)
H19	0.4912 (18)	0.9621 (13)	−0.1228 (11)	0.040 (4)*
C20	0.29701 (17)	0.96691 (11)	−0.03676 (9)	0.0311 (3)
H20	0.2361 (19)	1.0421 (15)	−0.0736 (11)	0.048 (5)*
C21	0.23330 (15)	0.90881 (10)	0.04282 (9)	0.0264 (3)
H21	0.1283 (17)	0.9397 (12)	0.0645 (10)	0.032 (4)*
C22	0.31651 (13)	0.80461 (10)	0.09334 (8)	0.0197 (2)
H22	0.2682 (15)	0.7666 (11)	0.1492 (9)	0.018 (3)*
O3	0.93894 (9)	0.15756 (7)	0.74756 (5)	0.02053 (18)
O4	1.08049 (9)	0.12056 (7)	0.48298 (5)	0.01794 (17)
N3	1.02428 (10)	0.16291 (7)	0.60887 (6)	0.01483 (19)
N4	0.97167 (11)	0.00894 (8)	0.60916 (6)	0.01509 (19)
H4	0.9496 (16)	−0.0385 (12)	0.5869 (10)	0.028 (4)*
C23	0.90976 (12)	0.01422 (9)	0.69460 (7)	0.0142 (2)
C24	0.95666 (12)	0.11981 (9)	0.69016 (7)	0.0151 (2)
C25	1.02959 (12)	0.09768 (9)	0.55874 (7)	0.0142 (2)
C26	1.07362 (13)	0.26901 (9)	0.57491 (8)	0.0170 (2)
H26A	1.0927 (14)	0.2804 (10)	0.6279 (8)	0.013 (3)*
H26B	1.1744 (16)	0.2570 (11)	0.5407 (9)	0.023 (3)*
C27	0.94845 (13)	0.36346 (9)	0.52373 (7)	0.0165 (2)
C28	0.81106 (13)	0.40374 (10)	0.56648 (8)	0.0202 (2)
H28	0.7967 (15)	0.3732 (11)	0.6300 (9)	0.022 (3)*
C29	0.69381 (14)	0.48924 (10)	0.52008 (9)	0.0249 (3)
H29	0.5967 (18)	0.5154 (13)	0.5524 (10)	0.035 (4)*
C30	0.71236 (15)	0.53480 (10)	0.43050 (9)	0.0263 (3)
H30	0.6324 (17)	0.5932 (13)	0.3983 (10)	0.034 (4)*
C31	0.84781 (15)	0.49567 (10)	0.38734 (9)	0.0263 (3)
H31	0.8640 (17)	0.5277 (12)	0.3241 (10)	0.032 (4)*
C32	0.96564 (14)	0.41008 (10)	0.43409 (8)	0.0218 (2)
H32	1.0621 (16)	0.3829 (11)	0.4053 (9)	0.022 (3)*
C34	0.62781 (13)	0.13002 (10)	0.69994 (8)	0.0190 (2)
C33	0.73129 (12)	0.02977 (9)	0.70213 (7)	0.0154 (2)
H34	0.6690 (16)	0.1930 (12)	0.6980 (9)	0.026 (4)*
C35	0.46692 (13)	0.14080 (10)	0.70126 (8)	0.0225 (3)
H35	0.3947 (16)	0.2127 (12)	0.6996 (9)	0.029 (4)*
C36	0.40973 (14)	0.05239 (11)	0.70489 (8)	0.0240 (3)
H36	0.2969 (17)	0.0578 (12)	0.7054 (9)	0.029 (4)*
C37	0.51247 (14)	−0.04803 (11)	0.70741 (9)	0.0261 (3)
H37	0.4742 (17)	−0.1106 (13)	0.7111 (10)	0.033 (4)*
C38	0.67266 (13)	−0.05915 (10)	0.70605 (8)	0.0217 (2)
H38	0.7440 (15)	−0.1331 (11)	0.7076 (9)	0.022 (3)*
C39	0.99171 (12)	−0.08471 (9)	0.76898 (7)	0.0157 (2)
C40	0.92049 (14)	−0.11020 (11)	0.85220 (8)	0.0237 (3)
H40	0.8138 (18)	−0.0666 (13)	0.8619 (10)	0.038 (4)*
C41	0.99948 (16)	−0.19464 (12)	0.92151 (9)	0.0297 (3)
H41	0.9464 (19)	−0.2089 (14)	0.9773 (11)	0.042 (4)*
C42	1.15024 (16)	−0.25295 (11)	0.90813 (9)	0.0281 (3)
H42	1.2059 (17)	−0.3099 (13)	0.9576 (10)	0.034 (4)*

C43	1.22097 (15)	−0.22835 (11)	0.82558 (9)	0.0286 (3)
H43	1.3276 (19)	−0.2691 (14)	0.8144 (11)	0.043 (4)*
C44	1.14211 (13)	−0.14453 (10)	0.75585 (8)	0.0223 (3)
H44	1.1949 (17)	−0.1309 (13)	0.6975 (10)	0.037 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0268 (4)	0.0196 (4)	0.0143 (4)	−0.0054 (3)	0.0002 (3)	−0.0068 (3)
O2	0.0239 (4)	0.0199 (4)	0.0184 (4)	−0.0089 (3)	−0.0015 (3)	−0.0071 (3)
N1	0.0163 (4)	0.0155 (4)	0.0130 (5)	−0.0044 (3)	−0.0001 (3)	−0.0035 (4)
N2	0.0200 (5)	0.0186 (5)	0.0136 (5)	−0.0079 (4)	0.0016 (4)	−0.0071 (4)
C1	0.0171 (5)	0.0144 (5)	0.0126 (5)	−0.0043 (4)	−0.0007 (4)	−0.0049 (4)
C2	0.0141 (5)	0.0156 (5)	0.0133 (5)	−0.0020 (4)	−0.0017 (4)	−0.0040 (4)
C3	0.0135 (5)	0.0156 (5)	0.0147 (5)	−0.0015 (4)	−0.0025 (4)	−0.0050 (4)
C4	0.0158 (5)	0.0182 (5)	0.0147 (5)	−0.0057 (4)	0.0005 (4)	−0.0022 (4)
C5	0.0196 (5)	0.0146 (5)	0.0114 (5)	−0.0025 (4)	0.0001 (4)	−0.0041 (4)
C6	0.0227 (6)	0.0195 (5)	0.0219 (6)	−0.0058 (5)	−0.0045 (5)	−0.0039 (5)
C7	0.0246 (6)	0.0268 (6)	0.0270 (7)	−0.0011 (5)	−0.0109 (5)	−0.0067 (5)
C8	0.0349 (7)	0.0219 (6)	0.0177 (6)	0.0032 (5)	−0.0083 (5)	−0.0036 (5)
C9	0.0340 (7)	0.0169 (5)	0.0181 (6)	−0.0044 (5)	0.0025 (5)	−0.0011 (5)
C10	0.0216 (5)	0.0175 (5)	0.0182 (6)	−0.0047 (4)	0.0017 (4)	−0.0058 (5)
C11	0.0168 (5)	0.0174 (5)	0.0121 (5)	−0.0058 (4)	−0.0014 (4)	−0.0011 (4)
C12	0.0204 (6)	0.0203 (6)	0.0269 (7)	−0.0034 (5)	−0.0029 (5)	−0.0065 (5)
C13	0.0192 (6)	0.0248 (6)	0.0349 (8)	−0.0013 (5)	−0.0029 (5)	−0.0040 (6)
C14	0.0202 (6)	0.0312 (7)	0.0254 (7)	−0.0106 (5)	−0.0083 (5)	0.0034 (5)
C15	0.0294 (6)	0.0252 (6)	0.0183 (6)	−0.0142 (5)	−0.0067 (5)	0.0006 (5)
C16	0.0231 (5)	0.0201 (5)	0.0142 (5)	−0.0078 (5)	−0.0010 (4)	−0.0037 (5)
C17	0.0179 (5)	0.0156 (5)	0.0150 (5)	−0.0044 (4)	−0.0030 (4)	−0.0042 (4)
C18	0.0244 (6)	0.0256 (6)	0.0169 (6)	−0.0048 (5)	−0.0005 (5)	−0.0020 (5)
C19	0.0342 (7)	0.0282 (7)	0.0198 (7)	−0.0084 (6)	−0.0034 (5)	0.0041 (5)
C20	0.0350 (7)	0.0193 (6)	0.0304 (7)	−0.0010 (5)	−0.0103 (6)	0.0004 (5)
C21	0.0238 (6)	0.0205 (6)	0.0314 (7)	0.0001 (5)	−0.0035 (5)	−0.0082 (5)
C22	0.0202 (5)	0.0187 (5)	0.0196 (6)	−0.0050 (4)	−0.0001 (4)	−0.0061 (5)
O3	0.0254 (4)	0.0232 (4)	0.0177 (4)	−0.0090 (3)	0.0012 (3)	−0.0110 (4)
O4	0.0209 (4)	0.0201 (4)	0.0137 (4)	−0.0082 (3)	0.0022 (3)	−0.0059 (3)
N3	0.0171 (4)	0.0144 (4)	0.0141 (5)	−0.0055 (3)	0.0001 (3)	−0.0053 (4)
N4	0.0188 (4)	0.0156 (4)	0.0122 (5)	−0.0063 (4)	0.0012 (3)	−0.0055 (4)
C23	0.0160 (5)	0.0145 (5)	0.0120 (5)	−0.0035 (4)	0.0004 (4)	−0.0051 (4)
C24	0.0141 (5)	0.0162 (5)	0.0148 (5)	−0.0032 (4)	−0.0012 (4)	−0.0053 (4)
C25	0.0122 (4)	0.0156 (5)	0.0146 (5)	−0.0025 (4)	−0.0018 (4)	−0.0051 (4)
C26	0.0171 (5)	0.0153 (5)	0.0200 (6)	−0.0071 (4)	−0.0001 (4)	−0.0057 (4)
C27	0.0189 (5)	0.0144 (5)	0.0185 (6)	−0.0072 (4)	−0.0014 (4)	−0.0061 (4)
C28	0.0220 (6)	0.0207 (6)	0.0194 (6)	−0.0058 (5)	−0.0005 (5)	−0.0085 (5)
C29	0.0218 (6)	0.0224 (6)	0.0319 (7)	−0.0024 (5)	−0.0029 (5)	−0.0123 (5)
C30	0.0285 (6)	0.0171 (5)	0.0325 (7)	−0.0066 (5)	−0.0102 (5)	−0.0036 (5)
C31	0.0344 (7)	0.0212 (6)	0.0204 (6)	−0.0116 (5)	−0.0037 (5)	0.0003 (5)
C32	0.0247 (6)	0.0194 (5)	0.0208 (6)	−0.0096 (5)	0.0029 (5)	−0.0052 (5)

C34	0.0209 (5)	0.0176 (5)	0.0173 (6)	−0.0042 (4)	−0.0004 (4)	−0.0054 (5)
C33	0.0155 (5)	0.0175 (5)	0.0123 (5)	−0.0033 (4)	−0.0008 (4)	−0.0046 (4)
C35	0.0195 (5)	0.0235 (6)	0.0189 (6)	0.0011 (5)	−0.0016 (4)	−0.0053 (5)
C36	0.0165 (5)	0.0330 (7)	0.0226 (6)	−0.0052 (5)	−0.0020 (4)	−0.0099 (5)
C37	0.0211 (6)	0.0312 (7)	0.0328 (7)	−0.0110 (5)	0.0021 (5)	−0.0169 (6)
C38	0.0195 (5)	0.0217 (6)	0.0264 (6)	−0.0055 (5)	0.0006 (5)	−0.0117 (5)
C39	0.0170 (5)	0.0157 (5)	0.0145 (5)	−0.0060 (4)	−0.0017 (4)	−0.0037 (4)
C40	0.0225 (6)	0.0267 (6)	0.0170 (6)	−0.0018 (5)	0.0008 (5)	−0.0055 (5)
C41	0.0329 (7)	0.0331 (7)	0.0148 (6)	−0.0036 (6)	−0.0014 (5)	−0.0022 (5)
C42	0.0321 (7)	0.0229 (6)	0.0227 (7)	−0.0021 (5)	−0.0100 (5)	−0.0005 (5)
C43	0.0231 (6)	0.0238 (6)	0.0295 (7)	0.0012 (5)	−0.0036 (5)	−0.0027 (5)
C44	0.0193 (5)	0.0215 (6)	0.0213 (6)	−0.0025 (5)	0.0016 (5)	−0.0048 (5)

Geometric parameters (Å, º)

O1—C2	1.2106 (13)	O3—C24	1.2105 (13)
O2—C3	1.2242 (13)	O4—C25	1.2256 (13)
N1—C2	1.3734 (14)	N3—C24	1.3700 (14)
N1—C3	1.4041 (14)	N3—C25	1.4017 (14)
N1—C4	1.4586 (14)	N3—C26	1.4691 (14)
N2—C3	1.3431 (14)	N4—C25	1.3458 (14)
N2—C1	1.4609 (14)	N4—C23	1.4663 (13)
N2—H2	0.918 (16)	N4—H4	0.916 (15)
C1—C17	1.5296 (14)	C23—C39	1.5282 (15)
C1—C11	1.5333 (15)	C23—C33	1.5347 (15)
C1—C2	1.5423 (15)	C23—C24	1.5420 (15)
C4—C5	1.5099 (15)	C26—C27	1.5089 (15)
C4—H4A	0.993 (14)	C26—H26A	0.998 (13)
C4—H4B	1.015 (13)	C26—H26B	0.993 (14)
C5—C6	1.3895 (16)	C27—C32	1.3883 (17)
C5—C10	1.3948 (16)	C27—C28	1.3959 (16)
C6—C7	1.3936 (17)	C28—C29	1.3877 (16)
C6—H6	1.001 (16)	C28—H28	0.983 (14)
C7—C8	1.3885 (19)	C29—C30	1.3872 (19)
C7—H7	0.967 (18)	C29—H29	0.995 (15)
C8—C9	1.3820 (19)	C30—C31	1.3824 (19)
C8—H8	0.985 (15)	C30—H30	0.950 (15)
C9—C10	1.3875 (17)	C31—C32	1.3935 (17)
C9—H9	0.990 (16)	C31—H31	0.981 (16)
C10—H10	0.951 (15)	C32—H32	0.965 (14)
C11—C12	1.3883 (15)	C34—C33	1.3904 (15)
C11—C16	1.3931 (16)	C34—C35	1.3957 (16)
C12—C13	1.3961 (17)	C34—H34	0.989 (15)
C12—H12	0.982 (15)	C33—C38	1.3919 (16)
C13—C14	1.3787 (19)	C35—C36	1.3795 (18)
C13—H13	0.993 (15)	C35—H35	0.990 (14)
C14—C15	1.3910 (19)	C36—C37	1.3882 (17)
C14—H14	0.973 (15)	C36—H36	0.985 (14)

C15—C16	1.3871 (17)	C37—C38	1.3888 (16)
C15—H15	0.978 (15)	C37—H37	0.959 (16)
C16—H16	1.005 (13)	C38—H38	1.009 (13)
C17—C22	1.3908 (15)	C39—C44	1.3899 (15)
C17—C18	1.3943 (16)	C39—C40	1.3900 (16)
C18—C19	1.3839 (17)	C40—C41	1.3929 (17)
C18—H18	1.008 (14)	C40—H40	0.993 (15)
C19—C20	1.389 (2)	C41—C42	1.3860 (18)
C19—H19	0.983 (17)	C41—H41	0.951 (17)
C20—C21	1.3823 (19)	C42—C43	1.3791 (19)
C20—H20	1.009 (17)	C42—H42	0.977 (15)
C21—C22	1.3919 (16)	C43—C44	1.3939 (17)
C21—H21	0.985 (15)	C43—H43	0.984 (16)
C22—H22	0.973 (13)	C44—H44	0.986 (16)
C2—N1—C3	111.64 (9)	C24—N3—C25	111.59 (9)
C2—N1—C4	124.66 (9)	C24—N3—C26	124.84 (9)
C3—N1—C4	123.46 (9)	C25—N3—C26	123.38 (9)
C3—N2—C1	113.00 (9)	C25—N4—C23	112.94 (9)
C3—N2—H2	120.6 (10)	C25—N4—H4	121.9 (9)
C1—N2—H2	125.0 (10)	C23—N4—H4	123.2 (9)
N2—C1—C17	109.90 (9)	N4—C23—C39	112.81 (8)
N2—C1—C11	112.56 (8)	N4—C23—C33	109.64 (8)
C17—C1—C11	112.87 (9)	C39—C23—C33	113.22 (9)
N2—C1—C2	100.97 (9)	N4—C23—C24	100.50 (8)
C17—C1—C2	112.28 (8)	C39—C23—C24	108.32 (9)
C11—C1—C2	107.66 (8)	C33—C23—C24	111.65 (8)
O1—C2—N1	126.04 (10)	O3—C24—N3	126.04 (10)
O1—C2—C1	127.35 (10)	O3—C24—C23	126.87 (10)
N1—C2—C1	106.60 (9)	N3—C24—C23	107.09 (9)
O2—C3—N2	128.73 (11)	O4—C25—N4	128.38 (10)
O2—C3—N1	123.75 (10)	O4—C25—N3	124.03 (10)
N2—C3—N1	107.51 (9)	N4—C25—N3	107.59 (9)
N1—C4—C5	114.99 (9)	N3—C26—C27	111.43 (9)
N1—C4—H4A	106.2 (8)	N3—C26—H26A	103.9 (7)
C5—C4—H4A	111.3 (8)	C27—C26—H26A	111.4 (7)
N1—C4—H4B	107.8 (8)	N3—C26—H26B	107.1 (8)
C5—C4—H4B	109.6 (7)	C27—C26—H26B	113.4 (8)
H4A—C4—H4B	106.5 (11)	H26A—C26—H26B	109.1 (11)
C6—C5—C10	119.12 (10)	C32—C27—C28	118.94 (11)
C6—C5—C4	122.60 (10)	C32—C27—C26	121.17 (10)
C10—C5—C4	118.14 (10)	C28—C27—C26	119.88 (10)
C5—C6—C7	120.13 (12)	C29—C28—C27	120.50 (12)
C5—C6—H6	119.7 (8)	C29—C28—H28	118.9 (7)
C7—C6—H6	120.1 (8)	C27—C28—H28	120.6 (7)
C8—C7—C6	120.31 (12)	C30—C29—C28	119.94 (11)
C8—C7—H7	120.1 (10)	C30—C29—H29	121.5 (9)
C6—C7—H7	119.6 (10)	C28—C29—H29	118.5 (9)

C9—C8—C7	119.67 (11)	C31—C30—C29	120.16 (12)
C9—C8—H8	120.5 (9)	C31—C30—H30	119.4 (9)
C7—C8—H8	119.8 (9)	C29—C30—H30	120.4 (9)
C8—C9—C10	120.23 (12)	C30—C31—C32	119.80 (12)
C8—C9—H9	118.6 (9)	C30—C31—H31	121.4 (8)
C10—C9—H9	121.2 (9)	C32—C31—H31	118.8 (8)
C9—C10—C5	120.53 (11)	C27—C32—C31	120.66 (11)
C9—C10—H10	118.3 (9)	C27—C32—H32	118.3 (8)
C5—C10—H10	121.1 (9)	C31—C32—H32	121.1 (8)
C12—C11—C16	119.64 (11)	C33—C34—C35	119.93 (11)
C12—C11—C1	121.58 (10)	C33—C34—H34	119.6 (8)
C16—C11—C1	118.72 (9)	C35—C34—H34	120.5 (8)
C11—C12—C13	120.00 (12)	C34—C33—C38	119.35 (10)
C11—C12—H12	120.6 (8)	C34—C33—C23	122.86 (10)
C13—C12—H12	119.4 (8)	C38—C33—C23	117.67 (9)
C14—C13—C12	119.98 (12)	C36—C35—C34	120.38 (11)
C14—C13—H13	119.8 (9)	C36—C35—H35	120.6 (8)
C12—C13—H13	120.2 (9)	C34—C35—H35	119.0 (8)
C13—C14—C15	120.38 (11)	C35—C36—C37	119.94 (11)
C13—C14—H14	117.6 (9)	C35—C36—H36	122.2 (8)
C15—C14—H14	122.0 (9)	C37—C36—H36	117.9 (8)
C16—C15—C14	119.69 (12)	C36—C37—C38	119.91 (12)
C16—C15—H15	119.8 (8)	C36—C37—H37	120.8 (8)
C14—C15—H15	120.5 (8)	C38—C37—H37	119.3 (8)
C15—C16—C11	120.30 (11)	C37—C38—C33	120.49 (11)
C15—C16—H16	120.7 (8)	C37—C38—H38	117.8 (8)
C11—C16—H16	119.0 (8)	C33—C38—H38	121.7 (8)
C22—C17—C18	119.23 (10)	C44—C39—C40	119.25 (10)
C22—C17—C1	122.18 (10)	C44—C39—C23	120.75 (10)
C18—C17—C1	118.43 (9)	C40—C39—C23	119.82 (9)
C19—C18—C17	120.52 (11)	C39—C40—C41	120.20 (11)
C19—C18—H18	120.1 (8)	C39—C40—H40	119.4 (9)
C17—C18—H18	119.3 (8)	C41—C40—H40	120.4 (9)
C18—C19—C20	119.97 (12)	C42—C41—C40	120.24 (12)
C18—C19—H19	119.5 (9)	C42—C41—H41	122.5 (10)
C20—C19—H19	120.5 (9)	C40—C41—H41	117.3 (10)
C21—C20—C19	119.90 (12)	C43—C42—C41	119.73 (12)
C21—C20—H20	120.2 (10)	C43—C42—H42	120.8 (9)
C19—C20—H20	119.9 (10)	C41—C42—H42	119.4 (9)
C20—C21—C22	120.26 (12)	C42—C43—C44	120.30 (11)
C20—C21—H21	120.9 (9)	C42—C43—H43	121.2 (10)
C22—C21—H21	118.8 (9)	C44—C43—H43	118.5 (10)
C17—C22—C21	120.10 (12)	C39—C44—C43	120.26 (11)
C17—C22—H22	122.1 (7)	C39—C44—H44	121.6 (9)
C21—C22—H22	117.8 (7)	C43—C44—H44	118.1 (9)
C3—N2—C1—C17	−114.96 (10)	C25—N4—C23—C39	−120.60 (10)
C3—N2—C1—C11	118.31 (10)	C25—N4—C23—C33	112.22 (10)

C3—N2—C1—C2	3.78 (11)	C25—N4—C23—C24	−5.46 (11)
C3—N1—C2—O1	177.87 (10)	C25—N3—C24—O3	178.72 (10)
C4—N1—C2—O1	3.27 (16)	C26—N3—C24—O3	−6.11 (17)
C3—N1—C2—C1	−2.49 (11)	C25—N3—C24—C23	−0.65 (11)
C4—N1—C2—C1	−177.09 (9)	C26—N3—C24—C23	174.52 (9)
N2—C1—C2—O1	178.98 (10)	N4—C23—C24—O3	−175.88 (10)
C17—C1—C2—O1	−64.02 (14)	C39—C23—C24—O3	−57.40 (14)
C11—C1—C2—O1	60.83 (13)	C33—C23—C24—O3	67.93 (14)
N2—C1—C2—N1	−0.65 (10)	N4—C23—C24—N3	3.48 (10)
C17—C1—C2—N1	116.35 (9)	C39—C23—C24—N3	121.96 (9)
C11—C1—C2—N1	−118.81 (9)	C33—C23—C24—N3	−112.71 (9)
C1—N2—C3—O2	174.03 (10)	C23—N4—C25—O4	−175.29 (10)
C1—N2—C3—N1	−5.44 (12)	C23—N4—C25—N3	5.39 (12)
C2—N1—C3—O2	−174.58 (10)	C24—N3—C25—O4	177.82 (9)
C4—N1—C3—O2	0.09 (16)	C26—N3—C25—O4	2.57 (16)
C2—N1—C3—N2	4.92 (12)	C24—N3—C25—N4	−2.82 (12)
C4—N1—C3—N2	179.59 (9)	C26—N3—C25—N4	−178.07 (9)
C2—N1—C4—C5	−87.88 (12)	C24—N3—C26—C27	−95.07 (12)
C3—N1—C4—C5	98.14 (12)	C25—N3—C26—C27	79.55 (12)
N1—C4—C5—C6	26.89 (15)	N3—C26—C27—C32	−107.67 (12)
N1—C4—C5—C10	−157.39 (10)	N3—C26—C27—C28	70.96 (13)
C10—C5—C6—C7	0.13 (17)	C32—C27—C28—C29	−0.20 (17)
C4—C5—C6—C7	175.80 (11)	C26—C27—C28—C29	−178.86 (11)
C5—C6—C7—C8	−0.21 (19)	C27—C28—C29—C30	0.40 (18)
C6—C7—C8—C9	−0.05 (19)	C28—C29—C30—C31	−0.37 (19)
C7—C8—C9—C10	0.38 (19)	C29—C30—C31—C32	0.14 (19)
C8—C9—C10—C5	−0.47 (18)	C28—C27—C32—C31	−0.04 (18)
C6—C5—C10—C9	0.21 (17)	C26—C27—C32—C31	178.61 (11)
C4—C5—C10—C9	−175.66 (10)	C30—C31—C32—C27	0.06 (19)
N2—C1—C11—C12	−12.47 (15)	C35—C34—C33—C38	−0.31 (17)
C17—C1—C11—C12	−137.58 (11)	C35—C34—C33—C23	175.69 (10)
C2—C1—C11—C12	97.93 (12)	N4—C23—C33—C34	−107.02 (12)
N2—C1—C11—C16	170.28 (10)	C39—C23—C33—C34	126.03 (11)
C17—C1—C11—C16	45.17 (13)	C24—C23—C33—C34	3.45 (15)
C2—C1—C11—C16	−79.32 (12)	N4—C23—C33—C38	69.04 (13)
C16—C11—C12—C13	−0.44 (18)	C39—C23—C33—C38	−57.91 (13)
C1—C11—C12—C13	−177.67 (11)	C24—C23—C33—C38	179.52 (10)
C11—C12—C13—C14	0.4 (2)	C33—C34—C35—C36	0.12 (18)
C12—C13—C14—C15	0.2 (2)	C34—C35—C36—C37	0.12 (19)
C13—C14—C15—C16	−0.76 (19)	C35—C36—C37—C38	−0.2 (2)
C14—C15—C16—C11	0.70 (18)	C36—C37—C38—C33	−0.02 (19)
C12—C11—C16—C15	−0.10 (17)	C34—C33—C38—C37	0.26 (18)
C1—C11—C16—C15	177.20 (10)	C23—C33—C38—C37	−175.94 (11)
N2—C1—C17—C22	100.75 (12)	N4—C23—C39—C44	23.53 (15)
C11—C1—C17—C22	−132.70 (11)	C33—C23—C39—C44	148.79 (11)
C2—C1—C17—C22	−10.78 (15)	C24—C23—C39—C44	−86.81 (12)
N2—C1—C17—C18	−74.61 (13)	N4—C23—C39—C40	−161.42 (10)
C11—C1—C17—C18	51.94 (14)	C33—C23—C39—C40	−36.16 (14)

C2—C1—C17—C18	173.85 (10)	C24—C23—C39—C40	88.24 (12)
C22—C17—C18—C19	−0.30 (19)	C44—C39—C40—C41	0.13 (19)
C1—C17—C18—C19	175.21 (12)	C23—C39—C40—C41	−174.99 (12)
C17—C18—C19—C20	−1.0 (2)	C39—C40—C41—C42	0.7 (2)
C18—C19—C20—C21	1.4 (2)	C40—C41—C42—C43	−1.1 (2)
C19—C20—C21—C22	−0.5 (2)	C41—C42—C43—C44	0.6 (2)
C18—C17—C22—C21	1.23 (18)	C40—C39—C44—C43	−0.63 (19)
C1—C17—C22—C21	−174.10 (11)	C23—C39—C44—C43	174.45 (11)
C20—C21—C22—C17	−0.9 (2)	C42—C43—C44—C39	0.3 (2)

Hydrogen-bond geometry (Å, º)

Cg3 and Cg7 are the centroids of the C11–C16 and C33–C38 phenyl rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O2^{i}	0.918 (16)	1.930 (16)	2.8446 (13)	173.3 (14)
N4—H4···O4^{ii}	0.916 (15)	1.958 (15)	2.8613 (12)	168.3 (14)
C8—H8···*Cg*7	0.985 (16)	2.987 (16)	3.5734 (14)	119.3 (11)
C15—H15···O3^{iii}	0.978 (15)	2.451 (16)	3.3830 (17)	159.2 (13)
C19—H19···*Cg*7^{iv}	0.983 (17)	2.732 (17)	3.6805 (15)	162.4 (14)
C22—H22···O3^{v}	0.973 (13)	2.586 (14)	3.3111 (15)	131.4 (11)
C31—H31···*Cg*3	0.981 (16)	2.917 (15)	3.8944 (15)	174.2 (12)
C41—H41···*Cg*3^{vi}	0.951 (17)	2.830 (17)	3.6570 (15)	146.0 (15)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*; (ii) −*x*+2, −*y*, −*z*+1; (iii) −*x*+2, −*y*+1, −*z*+1; (iv) *x*, *y*+1, *z*−1; (v) −*x*+1, −*y*+1, −*z*+1; (vi) *x*, *y*−1, *z*+1.