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

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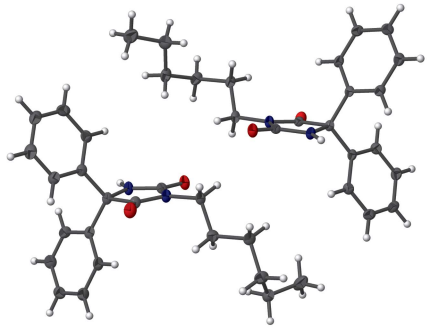
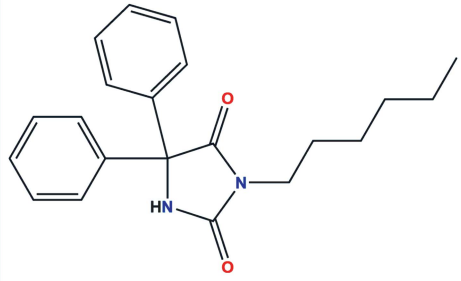
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title compound, $C_{21}H_{24}N_2O_2$, consists of two independent molecules differing primarily in the orientation of the ends of the hexyl substituent, the C—C—C—C torsion angles being 71.7 (3) and170.5 (2)°. In the crystal, each independent molecule forms a chain along the *a*-axis direction through a C—H···O hydrogen bond with one chain also including a C—H···π interaction. Paired N—H···O hydrogen bonds between independent molecules form ribbons with additional C—H···O hydrogen bonds and C—H···π(ring) interactions tying them into a three-dimensional structure.

3D view



Chemical scheme



Structure description

Hydantoin, a heterocycle containing two nitrogen atoms, is a nucleus found in numerous natural products and in several clinically important medicines. One of the most significant hydantoin derivatives is 5,5-diphenylimidazolidine-2,4-dione (phenytoin). As part of our ongoing studies of phenytoin derivatives (Ramli, Akrad *et al.*, 2017; Ramli, Guerrab *et al.*, 2017; Akrad *et al.*, 2017; Guerrab *et al.*, 2017*a*,*b*), the title compound was prepared and its crystal structure is reported here.

The asymmetric unit of the title compound consists of two independent molecules differing in the orientations of the substituents on the imidazolidine-2,4-dione ring (Fig. 1). Each imidazolidine-2,4-dione ring has two phenyl groups attached to the 5-position. The C10–C15 and C16–C21 phenyl rings are inclined to the C1/C2/N1/N2/C3 ring by 69.71 (12) and 71.80 (12)°, respectively, while the C31–C36 and C37–C42 phenyl rings make dihedral angles of 71.24 (11) and 67.85 (10)°, respectively, with the C22/C23/N3/C24/N4 ring. More significant are the different orientations of the ends of the *n*-hexyl chains with the C6—C7—C8—C9 torsion angle being 71.7 (3)° while the C27—C28—C29—C30 torsion angle is 170.5 (2)°.

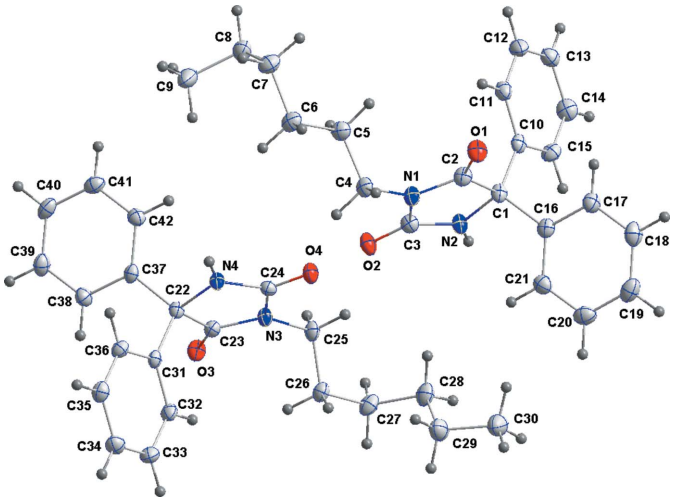


Figure 1
The asymmetric unit with labelling scheme and 50% probability ellipsoids.

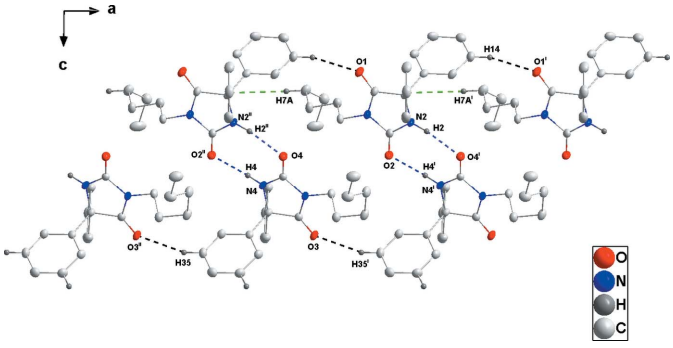


Figure 2
Detail of the chain-forming interactions. N—H···O and C—H···O hydrogen bonds are shown, respectively, as blue and black dashed lines. The C—H···π(ring) interactions are shown by green dashed lines [symmetry codes: (i) $x+1, y, z$; (ii) $-x+1, y, z$; (iii) $-x+1, -y+1, z$; (iv) $-x, -y, -z+1$].

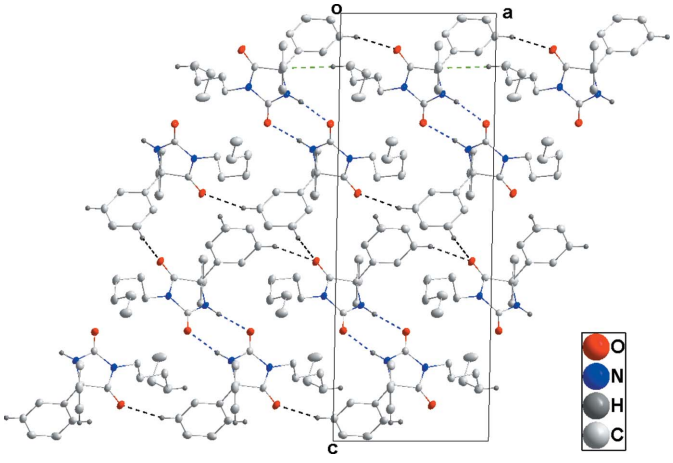


Figure 3
Packing viewed along the *b*-axis direction with intermolecular interactions depicted as in Fig. 2.

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

*Cg*3 is the centroid of the C16–C21 phenyl ring.

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O4^{i}	0.88	2.04	2.896 (2)	165
N4—H4···O2^{ii}	0.88	2.05	2.875 (2)	156
C14—H14···O1^{i}	0.95	2.44	3.370 (3)	165
C33—H33···O3^{iii}	0.95	2.48	3.413 (3)	169
C35—H35···O3^{ii}	0.95	2.45	3.363 (3)	161
C7—H7A···Cg3^{iv}	0.99	2.85	3.835 (3)	177

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{21}H_{24}N_2O_2$
M_r	336.42
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	100
a, b, c (Å)	8.5395 (13), 8.9377 (13), 23.444 (4)
β (°)	91.066 (2)
V (Å^3)	1789.0 (5)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.27 × 0.22 × 0.16
Data collection	
Diffractometer	Bruker *SMART APEX* CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.87, 0.99
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	34684, 9382, 7808
R_{int}	0.043
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.687
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.044, 0.112, 1.04
No. of reflections	9382
No. of parameters	454
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.35, −0.23

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

In the crystal, the O1-containing molecules form chains along the *a*-axis direction through a combination of C14—H14···O1 hydrogen bonds and C7—H7A···Cg3 interactions (Table 1 and Fig. 2; Cg3 is the centroid of phenyl ring C16–C21). O3-containing molecules form chains parallel to these through C35—H35···O3 hydrogen bonds. These chains are associated into ribbons by paired N2—H2···O4 and N4—H4···O2 hydrogen bonds (Table 1 and Fig. 2). Finally, C35—H35···O3 hydrogen bonds and additional C7—H7A···Cg3 interactions form a three-dimensional network (Table 1 and Fig. 3).

Synthesis and crystallization

To a solution of 5,5-diphenylimidazolidine-2,4-dione (1 g), one equivalent of hexyl bromide in absolute dimethylformamide

(DMF) was added and the resulting solution heated under reflux for 2 h in the presence of 1.3 equivalents of K_2CO_3. The reaction mixture was filtered while hot, and the solvent evaporated under reduced pressure. The residue obtained was dried and crystallized from an ethanol solution to yield colourless block-shaped single crystals of the title compound.

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2018). **3**, x180057 [https://doi.org/10.1107/S2414314618000573]

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Crystal data

$C_{21}H_{24}N_2O_2$
M_r = 336.42
Monoclinic, $P2_1$
a = 8.5395 (13) Å
b = 8.9377 (13) Å
c = 23.444 (4) Å
β = 91.066 (2)°
V = 1789.0 (5) Å^3
Z = 4
$F(000)$ = 720
D_x = 1.249 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9959 reflections
θ = 2.4–29.0°
μ = 0.08 mm^{-1}
T = 100 K
Block, colourless
0.27 × 0.22 × 0.16 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} = 0.87, T_{max} = 0.99
34684 measured reflections
9382 independent reflections
7808 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 29.2°, θ_{min} = 1.7°
h = −11→11
k = −12→12
l = −31→32

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.112
S = 1.04
9382 reflections
454 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0634P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Absolute structure: Refined as an inversion twin
Absolute structure parameter: 0.2 (10)

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 20 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. Refined as a 2-component inversion twin. H-atoms were placed in calculated positions (C—H = 0.95 - 0.99 Å; N—H = 0.88 Å). All were included as riding contributions with isotropic displacement parameters 1.2 - 1.5 times those of the attached atoms.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.36738 (17)	0.13246 (19)	0.08478 (6)	0.0250 (4)
O2	0.54242 (17)	−0.05628 (19)	0.25579 (6)	0.0235 (4)
N1	0.41641 (19)	0.0240 (2)	0.17241 (7)	0.0192 (4)
N2	0.6629 (2)	0.0916 (2)	0.18873 (7)	0.0194 (4)
H2	0.753310	0.105054	0.206598	0.023*
C1	0.6269 (2)	0.1530 (2)	0.13210 (8)	0.0173 (4)
C2	0.4539 (2)	0.1042 (3)	0.12497 (9)	0.0194 (4)
C3	0.5447 (2)	0.0128 (3)	0.21078 (8)	0.0186 (4)
C4	0.2645 (2)	−0.0477 (3)	0.18156 (9)	0.0199 (4)
H4A	0.179794	0.022126	0.169864	0.024*
H4B	0.253265	−0.068787	0.222740	0.024*
C5	0.2463 (3)	−0.1920 (3)	0.14840 (10)	0.0227 (5)
H5A	0.331597	−0.261481	0.159853	0.027*
H5B	0.256683	−0.170763	0.107196	0.027*
C6	0.0888 (2)	−0.2675 (3)	0.15827 (9)	0.0235 (5)
H6A	0.003576	−0.196276	0.148603	0.028*
H6B	0.080682	−0.293268	0.199174	0.028*
C7	0.0675 (3)	−0.4096 (3)	0.12246 (10)	0.0276 (5)
H7A	−0.043276	−0.441482	0.124454	0.033*
H7B	0.088694	−0.384982	0.082158	0.033*
C8	0.1711 (3)	−0.5404 (3)	0.14028 (10)	0.0266 (5)
H8A	0.167251	−0.617074	0.109820	0.032*
H8B	0.280678	−0.504984	0.144025	0.032*
C9	0.1242 (4)	−0.6123 (3)	0.19610 (10)	0.0419 (7)
H9A	0.196358	−0.694365	0.205375	0.063*
H9B	0.017325	−0.651426	0.192311	0.063*
H9C	0.128656	−0.537412	0.226628	0.063*
C10	0.7312 (2)	0.0792 (2)	0.08774 (8)	0.0180 (4)
C11	0.6759 (3)	−0.0238 (3)	0.04790 (8)	0.0233 (5)
H11	0.566983	−0.044721	0.045292	0.028*
C12	0.7783 (3)	−0.0967 (3)	0.01174 (9)	0.0281 (5)
H12	0.739177	−0.167693	−0.015100	0.034*
C13	0.9367 (3)	−0.0659 (3)	0.01483 (9)	0.0251 (5)
H13	1.006816	−0.116904	−0.009422	0.030*

C14	0.9931 (3)	0.0395 (3)	0.05343 (9)	0.0255 (5)
H14	1.101677	0.062665	0.054982	0.031*
C15	0.8914 (2)	0.1110 (3)	0.08962 (9)	0.0218 (5)
H15	0.930918	0.182710	0.116121	0.026*
C16	0.6343 (2)	0.3240 (3)	0.13026 (9)	0.0183 (4)
C17	0.6326 (3)	0.3966 (3)	0.07764 (9)	0.0226 (5)
H17	0.630919	0.339925	0.043366	0.027*
C18	0.6334 (3)	0.5521 (3)	0.07531 (10)	0.0272 (5)
H18	0.632310	0.601665	0.039448	0.033*
C19	0.6356 (3)	0.6347 (3)	0.12531 (10)	0.0270 (5)
H19	0.637703	0.740892	0.123583	0.032*
C20	0.6349 (3)	0.5640 (3)	0.17756 (10)	0.0268 (5)
H20	0.635423	0.621297	0.211695	0.032*
C21	0.6335 (3)	0.4083 (3)	0.18019 (9)	0.0225 (5)
H21	0.632013	0.359441	0.216169	0.027*
O3	0.12971 (17)	−0.14512 (18)	0.42033 (6)	0.0215 (3)
O4	−0.05315 (16)	0.08484 (18)	0.25818 (6)	0.0211 (3)
N3	0.07408 (19)	−0.0073 (2)	0.33947 (7)	0.0174 (4)
N4	−0.1652 (2)	−0.0900 (2)	0.31728 (7)	0.0171 (4)
H4	−0.251179	−0.108464	0.297218	0.020*
C22	−0.1303 (2)	−0.1580 (2)	0.37302 (8)	0.0156 (4)
C23	0.0409 (2)	−0.1062 (2)	0.38216 (8)	0.0165 (4)
C24	−0.0520 (2)	0.0039 (2)	0.30000 (8)	0.0159 (4)
C25	0.2227 (2)	0.0740 (3)	0.33453 (9)	0.0195 (4)
H25A	0.222194	0.128966	0.297854	0.023*
H25B	0.309686	0.000876	0.333843	0.023*
C26	0.2528 (2)	0.1844 (2)	0.38293 (9)	0.0209 (4)
H26A	0.249605	0.130812	0.419844	0.025*
H26B	0.168936	0.260940	0.382658	0.025*
C27	0.4117 (3)	0.2616 (3)	0.37742 (10)	0.0245 (5)
H27A	0.439694	0.308408	0.414494	0.029*
H27B	0.491579	0.184291	0.369658	0.029*
C28	0.4198 (3)	0.3809 (3)	0.33106 (10)	0.0260 (5)
H28A	0.529321	0.416227	0.328602	0.031*
H28B	0.390887	0.334628	0.293973	0.031*
C29	0.3142 (3)	0.5154 (3)	0.34056 (10)	0.0310 (5)
H29A	0.203536	0.483499	0.336361	0.037*
H29B	0.330425	0.552037	0.380079	0.037*
C30	0.3441 (3)	0.6422 (3)	0.29951 (10)	0.0360 (6)
H30A	0.268833	0.722907	0.306012	0.054*
H30B	0.332232	0.605846	0.260236	0.054*
H30C	0.450798	0.680161	0.305678	0.054*
C31	−0.2355 (2)	−0.0896 (2)	0.41845 (8)	0.0153 (4)
C32	−0.1822 (2)	0.0121 (3)	0.45902 (8)	0.0203 (4)
H32	−0.074698	0.039296	0.460449	0.024*
C33	−0.2851 (3)	0.0744 (3)	0.49763 (9)	0.0234 (5)
H33	−0.247891	0.144943	0.524997	0.028*
C34	−0.4416 (3)	0.0341 (3)	0.49632 (9)	0.0238 (5)

H34	−0.511559	0.076359	0.522925	0.029*
C35	−0.4958 (3)	−0.0679 (2)	0.45615 (9)	0.0217 (5)
H35	−0.603251	−0.095555	0.455181	0.026*
C36	−0.3939 (2)	−0.1296 (2)	0.41738 (9)	0.0190 (4)
H36	−0.431794	−0.199576	0.389908	0.023*
C37	−0.1370 (2)	−0.3279 (2)	0.37254 (9)	0.0166 (4)
C38	−0.1427 (2)	−0.4055 (3)	0.42411 (9)	0.0210 (5)
H38	−0.142967	−0.351269	0.458963	0.025*
C39	−0.1481 (3)	−0.5607 (3)	0.42524 (10)	0.0238 (5)
H39	−0.152122	−0.612256	0.460625	0.029*
C40	−0.1476 (3)	−0.6403 (3)	0.37429 (10)	0.0234 (5)
H40	−0.153488	−0.746382	0.374750	0.028*
C41	−0.1384 (3)	−0.5649 (3)	0.32287 (10)	0.0228 (5)
H41	−0.135478	−0.619557	0.288157	0.027*
C42	−0.1333 (2)	−0.4091 (3)	0.32185 (9)	0.0199 (5)
H42	−0.127420	−0.357978	0.286422	0.024*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0195 (8)	0.0308 (9)	0.0243 (8)	−0.0022 (7)	−0.0080 (6)	0.0069 (7)
O2	0.0190 (8)	0.0316 (9)	0.0200 (7)	−0.0027 (7)	−0.0016 (6)	0.0086 (7)
N1	0.0137 (8)	0.0232 (9)	0.0206 (8)	−0.0034 (8)	−0.0027 (6)	0.0039 (8)
N2	0.0138 (9)	0.0260 (10)	0.0181 (8)	−0.0035 (8)	−0.0046 (6)	0.0070 (7)
C1	0.0148 (11)	0.0199 (11)	0.0171 (9)	−0.0021 (8)	−0.0050 (8)	0.0048 (8)
C2	0.0148 (10)	0.0213 (11)	0.0219 (10)	−0.0003 (9)	−0.0038 (8)	0.0024 (9)
C3	0.0152 (10)	0.0211 (10)	0.0196 (9)	0.0011 (9)	−0.0008 (8)	0.0009 (9)
C4	0.0129 (10)	0.0241 (11)	0.0227 (9)	−0.0024 (8)	0.0003 (8)	0.0016 (9)
C5	0.0190 (11)	0.0246 (11)	0.0246 (10)	0.0001 (9)	0.0004 (8)	−0.0021 (9)
C6	0.0162 (10)	0.0248 (12)	0.0295 (11)	−0.0011 (9)	−0.0003 (8)	−0.0028 (9)
C7	0.0266 (12)	0.0268 (12)	0.0291 (11)	−0.0027 (10)	−0.0052 (9)	−0.0042 (10)
C8	0.0273 (12)	0.0232 (11)	0.0292 (11)	−0.0032 (10)	0.0023 (9)	−0.0003 (10)
C9	0.070 (2)	0.0289 (14)	0.0269 (12)	−0.0184 (14)	−0.0046 (12)	−0.0006 (11)
C10	0.0187 (10)	0.0181 (10)	0.0172 (9)	−0.0009 (9)	−0.0037 (8)	0.0057 (8)
C11	0.0213 (11)	0.0291 (12)	0.0194 (9)	−0.0079 (10)	−0.0014 (8)	0.0021 (9)
C12	0.0325 (13)	0.0312 (13)	0.0205 (10)	−0.0115 (11)	0.0006 (9)	−0.0041 (10)
C13	0.0278 (12)	0.0269 (12)	0.0206 (10)	0.0013 (10)	0.0023 (9)	0.0023 (9)
C14	0.0176 (11)	0.0311 (13)	0.0276 (11)	0.0012 (10)	−0.0028 (9)	0.0021 (10)
C15	0.0199 (11)	0.0221 (11)	0.0232 (10)	−0.0018 (9)	−0.0059 (8)	−0.0011 (9)
C16	0.0129 (11)	0.0207 (11)	0.0214 (10)	0.0000 (8)	−0.0028 (8)	0.0023 (8)
C17	0.0230 (12)	0.0222 (11)	0.0224 (11)	−0.0007 (10)	−0.0031 (9)	0.0032 (9)
C18	0.0249 (13)	0.0257 (13)	0.0310 (12)	0.0015 (10)	−0.0024 (10)	0.0092 (9)
C19	0.0200 (12)	0.0199 (12)	0.0413 (14)	0.0019 (10)	0.0011 (10)	0.0025 (10)
C20	0.0221 (12)	0.0287 (13)	0.0295 (12)	0.0014 (10)	0.0009 (9)	−0.0070 (10)
C21	0.0180 (11)	0.0279 (12)	0.0217 (10)	−0.0018 (10)	0.0007 (8)	−0.0004 (9)
O3	0.0167 (8)	0.0234 (8)	0.0242 (7)	−0.0007 (6)	−0.0066 (6)	0.0059 (6)
O4	0.0187 (7)	0.0242 (8)	0.0202 (7)	−0.0028 (6)	−0.0012 (6)	0.0065 (6)
N3	0.0125 (8)	0.0210 (9)	0.0186 (8)	−0.0034 (7)	−0.0021 (6)	0.0037 (7)

N4	0.0147 (9)	0.0205 (9)	0.0158 (8)	−0.0044 (7)	−0.0047 (6)	0.0036 (7)
C22	0.0149 (10)	0.0164 (10)	0.0155 (9)	−0.0011 (8)	−0.0028 (8)	0.0029 (8)
C23	0.0167 (10)	0.0154 (10)	0.0175 (9)	−0.0004 (9)	0.0002 (8)	0.0001 (8)
C24	0.0156 (10)	0.0174 (10)	0.0147 (8)	0.0005 (8)	−0.0003 (7)	−0.0007 (8)
C25	0.0148 (10)	0.0213 (11)	0.0225 (10)	−0.0037 (8)	0.0003 (8)	0.0034 (9)
C26	0.0186 (11)	0.0190 (10)	0.0251 (10)	−0.0025 (8)	−0.0003 (8)	0.0013 (8)
C27	0.0196 (11)	0.0220 (11)	0.0317 (11)	−0.0031 (9)	−0.0066 (9)	0.0012 (9)
C28	0.0188 (11)	0.0265 (12)	0.0327 (12)	−0.0055 (9)	−0.0018 (9)	0.0036 (10)
C29	0.0387 (14)	0.0269 (12)	0.0276 (11)	0.0010 (11)	0.0031 (10)	0.0046 (10)
C30	0.0512 (17)	0.0285 (13)	0.0283 (12)	−0.0048 (12)	−0.0017 (11)	0.0025 (10)
C31	0.0155 (10)	0.0138 (10)	0.0167 (9)	0.0000 (8)	−0.0010 (7)	0.0039 (8)
C32	0.0196 (11)	0.0205 (11)	0.0208 (9)	−0.0060 (9)	−0.0018 (8)	0.0003 (9)
C33	0.0273 (12)	0.0221 (11)	0.0209 (10)	−0.0046 (9)	−0.0014 (9)	−0.0034 (9)
C34	0.0245 (12)	0.0226 (11)	0.0243 (10)	0.0030 (9)	0.0026 (9)	−0.0004 (9)
C35	0.0161 (10)	0.0220 (11)	0.0269 (10)	−0.0007 (9)	−0.0008 (8)	0.0026 (9)
C36	0.0178 (10)	0.0179 (11)	0.0210 (10)	−0.0015 (9)	−0.0028 (8)	−0.0009 (8)
C37	0.0123 (11)	0.0161 (10)	0.0215 (10)	−0.0007 (8)	−0.0003 (8)	0.0026 (8)
C38	0.0224 (12)	0.0215 (11)	0.0190 (10)	0.0012 (10)	−0.0003 (8)	0.0030 (9)
C39	0.0236 (12)	0.0186 (11)	0.0294 (11)	0.0023 (9)	0.0020 (9)	0.0059 (9)
C40	0.0188 (12)	0.0157 (11)	0.0355 (12)	0.0000 (9)	−0.0003 (10)	−0.0009 (9)
C41	0.0188 (12)	0.0218 (12)	0.0278 (11)	−0.0005 (9)	−0.0009 (9)	−0.0053 (9)
C42	0.0187 (11)	0.0231 (11)	0.0178 (10)	−0.0014 (9)	−0.0011 (8)	0.0006 (9)

Geometric parameters (Å, º)

O1—C2	1.213 (2)	O3—C23	1.213 (2)
O2—C3	1.223 (2)	O4—C24	1.219 (2)
N1—C2	1.366 (3)	N3—C23	1.369 (3)
N1—C3	1.408 (2)	N3—C24	1.410 (2)
N1—C4	1.466 (3)	N3—C25	1.469 (3)
N2—C3	1.342 (3)	N4—C24	1.348 (3)
N2—C1	1.464 (2)	N4—C22	1.467 (2)
N2—H2	0.8800	N4—H4	0.8800
C1—C10	1.531 (3)	C22—C37	1.520 (3)
C1—C16	1.531 (3)	C22—C31	1.533 (3)
C1—C2	1.547 (3)	C22—C23	1.544 (3)
C4—C5	1.513 (3)	C25—C26	1.522 (3)
C4—H4A	0.9900	C25—H25A	0.9900
C4—H4B	0.9900	C25—H25B	0.9900
C5—C6	1.526 (3)	C26—C27	1.530 (3)
C5—H5A	0.9900	C26—H26A	0.9900
C5—H5B	0.9900	C26—H26B	0.9900
C6—C7	1.531 (3)	C27—C28	1.525 (3)
C6—H6A	0.9900	C27—H27A	0.9900
C6—H6B	0.9900	C27—H27B	0.9900
C7—C8	1.520 (3)	C28—C29	1.522 (3)
C7—H7A	0.9900	C28—H28A	0.9900
C7—H7B	0.9900	C28—H28B	0.9900

C8—C9	1.518 (3)	C29—C30	1.512 (3)
C8—H8A	0.9900	C29—H29A	0.9900
C8—H8B	0.9900	C29—H29B	0.9900
C9—H9A	0.9800	C30—H30A	0.9800
C9—H9B	0.9800	C30—H30B	0.9800
C9—H9C	0.9800	C30—H30C	0.9800
C10—C11	1.388 (3)	C31—C32	1.386 (3)
C10—C15	1.397 (3)	C31—C36	1.399 (3)
C11—C12	1.391 (3)	C32—C33	1.390 (3)
C11—H11	0.9500	C32—H32	0.9500
C12—C13	1.381 (3)	C33—C34	1.383 (3)
C12—H12	0.9500	C33—H33	0.9500
C13—C14	1.387 (3)	C34—C35	1.384 (3)
C13—H13	0.9500	C34—H34	0.9500
C14—C15	1.382 (3)	C35—C36	1.385 (3)
C14—H14	0.9500	C35—H35	0.9500
C15—H15	0.9500	C36—H36	0.9500
C16—C21	1.392 (3)	C37—C42	1.393 (3)
C16—C17	1.394 (3)	C37—C38	1.395 (3)
C17—C18	1.391 (3)	C38—C39	1.388 (3)
C17—H17	0.9500	C38—H38	0.9500
C18—C19	1.385 (3)	C39—C40	1.390 (3)
C18—H18	0.9500	C39—H39	0.9500
C19—C20	1.379 (3)	C40—C41	1.385 (3)
C19—H19	0.9500	C40—H40	0.9500
C20—C21	1.393 (4)	C41—C42	1.393 (3)
C20—H20	0.9500	C41—H41	0.9500
C21—H21	0.9500	C42—H42	0.9500

C2—N1—C3	111.46 (16)	C23—N3—C24	111.06 (16)
C2—N1—C4	124.74 (16)	C23—N3—C25	124.62 (16)
C3—N1—C4	123.75 (17)	C24—N3—C25	124.30 (17)
C3—N2—C1	113.56 (16)	C24—N4—C22	112.97 (16)
C3—N2—H2	123.2	C24—N4—H4	123.5
C1—N2—H2	123.2	C22—N4—H4	123.5
N2—C1—C10	109.88 (17)	N4—C22—C37	113.61 (17)
N2—C1—C16	113.07 (17)	N4—C22—C31	109.97 (16)
C10—C1—C16	112.73 (18)	C37—C22—C31	112.37 (17)
N2—C1—C2	100.15 (16)	N4—C22—C23	100.14 (16)
C10—C1—C2	111.81 (17)	C37—C22—C23	109.62 (17)
C16—C1—C2	108.54 (18)	C31—C22—C23	110.48 (17)
O1—C2—N1	126.36 (19)	O3—C23—N3	126.09 (19)
O1—C2—C1	126.3 (2)	O3—C23—C22	126.43 (19)
N1—C2—C1	107.32 (16)	N3—C23—C22	107.47 (16)
O2—C3—N2	128.42 (19)	O4—C24—N4	128.04 (18)
O2—C3—N1	124.22 (19)	O4—C24—N3	124.38 (19)
N2—C3—N1	107.36 (17)	N4—C24—N3	107.58 (17)
N1—C4—C5	112.31 (17)	N3—C25—C26	113.33 (17)

N1—C4—H4A	109.1	N3—C25—H25A	108.9
C5—C4—H4A	109.1	C26—C25—H25A	108.9
N1—C4—H4B	109.1	N3—C25—H25B	108.9
C5—C4—H4B	109.1	C26—C25—H25B	108.9
H4A—C4—H4B	107.9	H25A—C25—H25B	107.7
C4—C5—C6	112.39 (18)	C25—C26—C27	111.52 (18)
C4—C5—H5A	109.1	C25—C26—H26A	109.3
C6—C5—H5A	109.1	C27—C26—H26A	109.3
C4—C5—H5B	109.1	C25—C26—H26B	109.3
C6—C5—H5B	109.1	C27—C26—H26B	109.3
H5A—C5—H5B	107.9	H26A—C26—H26B	108.0
C5—C6—C7	112.30 (18)	C28—C27—C26	115.30 (18)
C5—C6—H6A	109.1	C28—C27—H27A	108.4
C7—C6—H6A	109.1	C26—C27—H27A	108.5
C5—C6—H6B	109.1	C28—C27—H27B	108.5
C7—C6—H6B	109.1	C26—C27—H27B	108.4
H6A—C6—H6B	107.9	H27A—C27—H27B	107.5
C8—C7—C6	115.12 (18)	C29—C28—C27	114.42 (19)
C8—C7—H7A	108.5	C29—C28—H28A	108.7
C6—C7—H7A	108.5	C27—C28—H28A	108.7
C8—C7—H7B	108.5	C29—C28—H28B	108.7
C6—C7—H7B	108.5	C27—C28—H28B	108.7
H7A—C7—H7B	107.5	H28A—C28—H28B	107.6
C9—C8—C7	113.6 (2)	C30—C29—C28	113.0 (2)
C9—C8—H8A	108.8	C30—C29—H29A	109.0
C7—C8—H8A	108.8	C28—C29—H29A	109.0
C9—C8—H8B	108.8	C30—C29—H29B	109.0
C7—C8—H8B	108.8	C28—C29—H29B	109.0
H8A—C8—H8B	107.7	H29A—C29—H29B	107.8
C8—C9—H9A	109.5	C29—C30—H30A	109.5
C8—C9—H9B	109.5	C29—C30—H30B	109.5
H9A—C9—H9B	109.5	H30A—C30—H30B	109.5
C8—C9—H9C	109.5	C29—C30—H30C	109.5
H9A—C9—H9C	109.5	H30A—C30—H30C	109.5
H9B—C9—H9C	109.5	H30B—C30—H30C	109.5
C11—C10—C15	118.4 (2)	C32—C31—C36	118.98 (19)
C11—C10—C1	123.27 (19)	C32—C31—C22	123.29 (18)
C15—C10—C1	118.18 (19)	C36—C31—C22	117.71 (18)
C10—C11—C12	120.8 (2)	C31—C32—C33	120.4 (2)
C10—C11—H11	119.6	C31—C32—H32	119.8
C12—C11—H11	119.6	C33—C32—H32	119.8
C13—C12—C11	120.0 (2)	C34—C33—C32	120.2 (2)
C13—C12—H12	120.0	C34—C33—H33	119.9
C11—C12—H12	120.0	C32—C33—H33	119.9
C12—C13—C14	119.8 (2)	C33—C34—C35	119.8 (2)
C12—C13—H13	120.1	C33—C34—H34	120.1
C14—C13—H13	120.1	C35—C34—H34	120.1
C15—C14—C13	120.0 (2)	C34—C35—C36	120.2 (2)

C15—C14—H14	120.0	C34—C35—H35	119.9
C13—C14—H14	120.0	C36—C35—H35	119.9
C14—C15—C10	120.8 (2)	C35—C36—C31	120.4 (2)
C14—C15—H15	119.6	C35—C36—H36	119.8
C10—C15—H15	119.6	C31—C36—H36	119.8
C21—C16—C17	119.5 (2)	C42—C37—C38	118.8 (2)
C21—C16—C1	121.0 (2)	C42—C37—C22	121.68 (19)
C17—C16—C1	119.4 (2)	C38—C37—C22	119.48 (19)
C18—C17—C16	120.0 (2)	C39—C38—C37	121.0 (2)
C18—C17—H17	120.0	C39—C38—H38	119.5
C16—C17—H17	120.0	C37—C38—H38	119.5
C19—C18—C17	119.9 (2)	C38—C39—C40	119.6 (2)
C19—C18—H18	120.0	C38—C39—H39	120.2
C17—C18—H18	120.0	C40—C39—H39	120.2
C20—C19—C18	120.5 (2)	C41—C40—C39	120.0 (2)
C20—C19—H19	119.8	C41—C40—H40	120.0
C18—C19—H19	119.8	C39—C40—H40	120.0
C19—C20—C21	119.8 (2)	C40—C41—C42	120.2 (2)
C19—C20—H20	120.1	C40—C41—H41	119.9
C21—C20—H20	120.1	C42—C41—H41	119.9
C16—C21—C20	120.2 (2)	C41—C42—C37	120.3 (2)
C16—C21—H21	119.9	C41—C42—H42	119.8
C20—C21—H21	119.9	C37—C42—H42	119.8

C3—N2—C1—C10	−114.0 (2)	C24—N4—C22—C37	−125.53 (19)
C3—N2—C1—C16	119.1 (2)	C24—N4—C22—C31	107.5 (2)
C3—N2—C1—C2	3.8 (2)	C24—N4—C22—C23	−8.8 (2)
C3—N1—C2—O1	−179.8 (2)	C24—N3—C23—O3	175.7 (2)
C4—N1—C2—O1	2.7 (4)	C25—N3—C23—O3	−3.0 (3)
C3—N1—C2—C1	−0.1 (2)	C24—N3—C23—C22	−4.8 (2)
C4—N1—C2—C1	−177.53 (19)	C25—N3—C23—C22	176.59 (18)
N2—C1—C2—O1	177.7 (2)	N4—C22—C23—O3	−172.6 (2)
C10—C1—C2—O1	−66.0 (3)	C37—C22—C23—O3	−52.9 (3)
C16—C1—C2—O1	59.0 (3)	C31—C22—C23—O3	71.5 (3)
N2—C1—C2—N1	−2.1 (2)	N4—C22—C23—N3	7.8 (2)
C10—C1—C2—N1	114.28 (19)	C37—C22—C23—N3	127.54 (18)
C16—C1—C2—N1	−120.8 (2)	C31—C22—C23—N3	−108.09 (18)
C1—N2—C3—O2	176.6 (2)	C22—N4—C24—O4	−173.8 (2)
C1—N2—C3—N1	−4.0 (3)	C22—N4—C24—N3	6.5 (2)
C2—N1—C3—O2	−178.2 (2)	C23—N3—C24—O4	179.5 (2)
C4—N1—C3—O2	−0.7 (3)	C25—N3—C24—O4	−1.9 (3)
C2—N1—C3—N2	2.5 (3)	C23—N3—C24—N4	−0.8 (2)
C4—N1—C3—N2	179.94 (19)	C25—N3—C24—N4	177.87 (18)
C2—N1—C4—C5	77.6 (3)	C23—N3—C25—C26	−65.2 (3)
C3—N1—C4—C5	−99.6 (2)	C24—N3—C25—C26	116.3 (2)
N1—C4—C5—C6	179.51 (17)	N3—C25—C26—C27	177.58 (17)
C4—C5—C6—C7	177.25 (18)	C25—C26—C27—C28	74.5 (2)
C5—C6—C7—C8	69.8 (3)	C26—C27—C28—C29	63.9 (3)

C6—C7—C8—C9	71.7 (3)	C27—C28—C29—C30	170.5 (2)
N2—C1—C10—C11	107.6 (2)	N4—C22—C31—C32	−105.6 (2)
C16—C1—C10—C11	−125.3 (2)	C37—C22—C31—C32	126.8 (2)
C2—C1—C10—C11	−2.6 (3)	C23—C22—C31—C32	4.0 (3)
N2—C1—C10—C15	−68.7 (2)	N4—C22—C31—C36	72.5 (2)
C16—C1—C10—C15	58.4 (2)	C37—C22—C31—C36	−55.1 (2)
C2—C1—C10—C15	−178.94 (18)	C23—C22—C31—C36	−177.84 (18)
C15—C10—C11—C12	1.7 (3)	C36—C31—C32—C33	−0.7 (3)
C1—C10—C11—C12	−174.5 (2)	C22—C31—C32—C33	177.4 (2)
C10—C11—C12—C13	−0.6 (3)	C31—C32—C33—C34	0.8 (3)
C11—C12—C13—C14	−1.0 (4)	C32—C33—C34—C35	−0.4 (3)
C12—C13—C14—C15	1.5 (3)	C33—C34—C35—C36	0.1 (3)
C13—C14—C15—C10	−0.4 (3)	C34—C35—C36—C31	0.0 (3)
C11—C10—C15—C14	−1.2 (3)	C32—C31—C36—C35	0.3 (3)
C1—C10—C15—C14	175.2 (2)	C22—C31—C36—C35	−177.90 (18)
N2—C1—C16—C21	−16.0 (3)	N4—C22—C37—C42	16.6 (3)
C10—C1—C16—C21	−141.4 (2)	C31—C22—C37—C42	142.31 (19)
C2—C1—C16—C21	94.2 (2)	C23—C22—C37—C42	−94.4 (2)
N2—C1—C16—C17	167.80 (18)	N4—C22—C37—C38	−165.08 (18)
C10—C1—C16—C17	42.4 (3)	C31—C22—C37—C38	−39.4 (3)
C2—C1—C16—C17	−82.0 (2)	C23—C22—C37—C38	83.8 (2)
C21—C16—C17—C18	1.3 (3)	C42—C37—C38—C39	−1.3 (3)
C1—C16—C17—C18	177.6 (2)	C22—C37—C38—C39	−179.7 (2)
C16—C17—C18—C19	−0.1 (4)	C37—C38—C39—C40	0.1 (4)
C17—C18—C19—C20	−0.9 (4)	C38—C39—C40—C41	1.4 (4)
C18—C19—C20—C21	0.7 (4)	C39—C40—C41—C42	−1.5 (4)
C17—C16—C21—C20	−1.6 (3)	C40—C41—C42—C37	0.2 (4)
C1—C16—C21—C20	−177.8 (2)	C38—C37—C42—C41	1.2 (3)
C19—C20—C21—C16	0.6 (4)	C22—C37—C42—C41	179.5 (2)

Hydrogen-bond geometry (Å, º)

Cg3 is the centroid of the C16–C21 phenyl ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O4^{i}	0.88	2.04	2.896 (2)	165
N4—H4···O2^{ii}	0.88	2.05	2.875 (2)	156
C14—H14···O1^{i}	0.95	2.44	3.370 (3)	165
C33—H33···O3^{iii}	0.95	2.48	3.413 (3)	169
C35—H35···O3^{ii}	0.95	2.45	3.363 (3)	161
C7—H7*A*···*Cg*3^{iv}	0.99	2.85	3.835 (3)	177

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