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3-*n*-Pentyl-5,5-diphenylimidazolidine-2,4-dione

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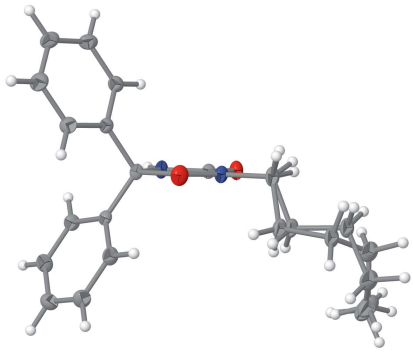
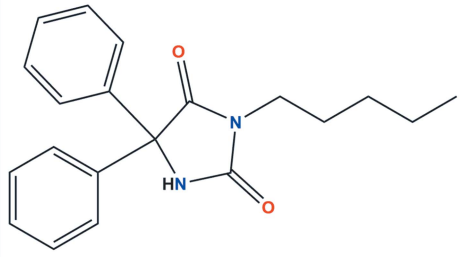
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{20}H_{22}N_2O_2$, the central five-membered imidazolidine ring makes dihedral angles of 63.85 (6) and 70.38 (6)° with the two substituent phenyl rings. In the crystal, molecules form an inversion dimer through a pair of N—H···O hydrogen bonds. These are linked into a three-dimensional network *via* C—H···O hydrogen bonds. The *n*-pentyl chain is disordered over two sites, with an occupancy ratio of 0.876 (2):0.124 (2).

3D view



Chemical scheme



Structure description

As part of our ongoing studies of 5,5-diphenylimidazolidine-2,4-dione 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 imidazolidine-2,4-dione ring has two phenyl groups attached at the 5-position (Fig. 1). The C4–C9 and C10–C15 rings are inclined to the five-membered ring by 70.38 (6) and 63.85 (6)°, respectively. In the crystal, a pair of N—H···O hydrogen bonds (N1—H1···O1^{i}; symmetry code as in Table 1) link the molecules into an inversion dimer. The dimers are further linked into a three-dimensional network *via* C—H···O hydrogen bonds (C12—H12···O2^{ii} and C14—H14···O2^{iii}; Table 1 and Fig. 2). The structure consists of channels running along the *a* axis and having an approximately oval cross-section of *ca* 16.8 × 7.8 Å^2 (Fig. 3).

Synthesis and crystallization

To a solution of 5,5-diphenylimidazolidine-2,4-dione (1 g, 3.96 mmol), one equivalent of pentyl bromide in absolute dimethylformamide (DMF) was added and the resulting solution heated under reflux for 3 h in the presence of 1.3 equivalents of K_2CO_3. The

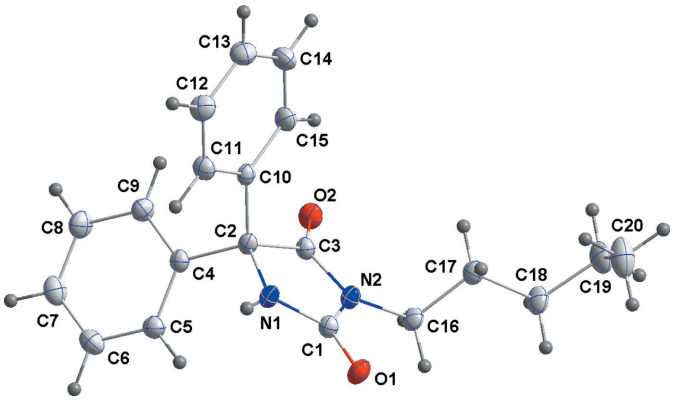


Figure 1
The molecular structure of the title compound, with the atom-labelling scheme and 50% probability displacement ellipsoids for non-H atoms. Only the major component of the disordered *n*-pentyl chain is shown.

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.

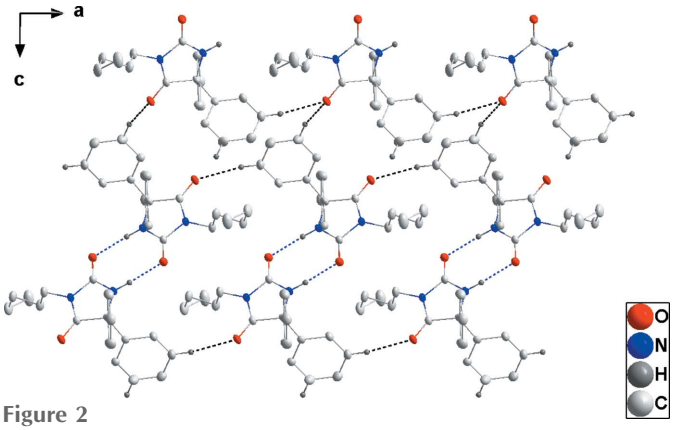


Figure 2
A packing diagram of the title compound, viewed along the *a* axis. N—H···O and C—H···O hydrogen bonds are shown as dashed lines. H atoms not involved in the interactions have been omitted.

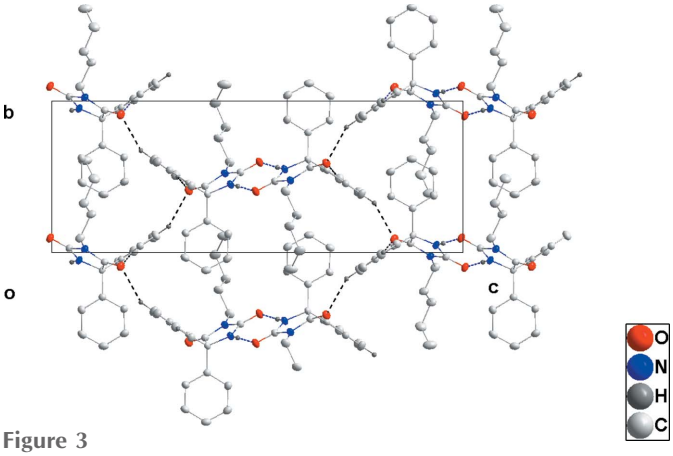


Figure 3
A packing diagram, viewed along the *b* axis, showing intermolecular interactions (dashed lines). One complete channel is shown in the lower centre of the drawing. H atoms not involved in the interactions have been omitted.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.884 (16)	1.972 (16)	2.8538 (12)	175.9 (15)
C12—H12···O2^{ii}	0.95	2.47	3.3960 (14)	166
C14—H14···O2^{iii}	0.95	2.56	3.4475 (15)	156

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x-1, y, z$; (iii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{22}N_2O_2$
M_r	322.39
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	100
a, *b*, *c* (Å)	8.5949 (9), 8.5931 (9), 23.276 (2)
β (°)	90.348 (2)
V (Å^3)	1719.1 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.46 × 0.43 × 0.13
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.91, 0.99
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	32274, 4644, 3849
R_{int}	0.032
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.688
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.047, 0.136, 1.10
No. of reflections	4644
No. of parameters	236
No. of restraints	8
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.54, −0.38

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

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The *n*-pentyl chain is disordered over two sites and the occupancy ratio was refined to 0.876 (2):0.124 (2). The geometries of the disordered components were restrained to be comparable. Constraints of the same anisotropic displacement parameters were also applied for the disordered non-H atoms.

Acknowledgements

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full crystallographic data

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3-*n*-Pentyl-5,5-diphenylimidazolidine-2,4-dione

Crystal data

$C_{20}H_{22}N_2O_2$
M_r = 322.39
Monoclinic, $P2_1/n$
a = 8.5949 (9) Å
b = 8.5931 (9) Å
c = 23.276 (2) Å
β = 90.348 (2)°
V = 1719.1 (3) Å^3
Z = 4
$F(000)$ = 688
D_x = 1.246 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9926 reflections
θ = 2.4–29.2°
μ = 0.08 mm^{-1}
T = 100 K
Plate, colourless
0.46 × 0.43 × 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} = 0.91, T_{max} = 0.99
32274 measured reflections
4644 independent reflections
3849 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 29.3°, θ_{min} = 1.8°
h = −11→11
k = −11→11
l = −31→31

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.136
S = 1.10
4644 reflections
236 parameters
8 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
$w = 1/[\sigma^2(F_o^2) + (0.0803P)^2 + 0.3238P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 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. H-atoms attached to carbon were placed in calculated positions (C—H = 0.95 - 0.99 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}	Occ. (<1)
O1	0.70156 (9)	0.59673 (10)	0.50462 (3)	0.02237 (19)	
O2	0.87704 (9)	0.41015 (10)	0.33272 (4)	0.02262 (19)	
N1	0.58128 (10)	0.44972 (11)	0.43413 (4)	0.0180 (2)	
H1	0.4913 (18)	0.4382 (18)	0.4518 (6)	0.027 (4)*	
N2	0.82575 (10)	0.52328 (11)	0.42027 (4)	0.0178 (2)	
C1	0.69930 (12)	0.52957 (12)	0.45825 (5)	0.0168 (2)	
C2	0.61887 (11)	0.38545 (12)	0.37780 (4)	0.0158 (2)	
C3	0.78989 (12)	0.43843 (12)	0.37198 (5)	0.0170 (2)	
C4	0.61088 (11)	0.20752 (12)	0.37723 (5)	0.0171 (2)	
C5	0.61400 (12)	0.12283 (13)	0.42812 (5)	0.0212 (2)	
H5	0.621107	0.175526	0.463921	0.025*	
C6	0.60671 (14)	−0.03919 (14)	0.42677 (5)	0.0254 (3)	
H6	0.609122	−0.096649	0.461635	0.030*	
C7	0.59598 (14)	−0.11648 (14)	0.37474 (6)	0.0262 (3)	
H7	0.588795	−0.226785	0.373962	0.031*	
C8	0.59569 (14)	−0.03291 (14)	0.32362 (6)	0.0257 (3)	
H8	0.590429	−0.086110	0.287885	0.031*	
C9	0.60312 (13)	0.12879 (13)	0.32486 (5)	0.0215 (2)	
H9	0.602914	0.185852	0.289907	0.026*	
C10	0.51272 (12)	0.45835 (12)	0.33207 (4)	0.0160 (2)	
C11	0.35237 (13)	0.44099 (13)	0.33893 (5)	0.0213 (2)	
H11	0.313738	0.380959	0.370002	0.026*	
C12	0.24873 (13)	0.51060 (15)	0.30077 (5)	0.0253 (2)	
H12	0.139838	0.498098	0.305787	0.030*	
C13	0.30454 (14)	0.59832 (15)	0.25538 (6)	0.0274 (3)	
H13	0.233993	0.647602	0.229603	0.033*	
C14	0.46365 (14)	0.61397 (15)	0.24768 (5)	0.0282 (3)	
H14	0.501879	0.672776	0.216217	0.034*	
C15	0.56768 (13)	0.54401 (14)	0.28578 (5)	0.0229 (2)	
H15	0.676517	0.554837	0.280135	0.027*	
C16	0.97712 (12)	0.59637 (14)	0.43206 (5)	0.0234 (2)	0.876 (2)
H16A	1.060263	0.526078	0.418348	0.028*	0.876 (2)
H16B	0.989924	0.607509	0.474154	0.028*	0.876 (2)
C17	0.99889 (15)	0.75387 (15)	0.40460 (7)	0.0243 (3)	0.876 (2)
H17A	0.912726	0.823496	0.416073	0.029*	0.876 (2)

H17B	0.995667	0.742857	0.362273	0.029*	0.876 (2)
C18	1.15373 (14)	0.82592 (16)	0.42272 (7)	0.0253 (3)	0.876 (2)
H18A	1.157565	0.833338	0.465144	0.030*	0.876 (2)
H18B	1.239395	0.756659	0.410473	0.030*	0.876 (2)
C19	1.17926 (16)	0.98717 (18)	0.39724 (7)	0.0315 (3)	0.876 (2)
H19A	1.170114	0.980564	0.354896	0.038*	0.876 (2)
H19B	1.286242	1.021956	0.406625	0.038*	0.876 (2)
C20	1.0637 (3)	1.1084 (2)	0.41924 (13)	0.0403 (5)	0.876 (2)
H20A	1.086008	1.209360	0.401548	0.061*	0.876 (2)
H20B	1.073526	1.117197	0.461086	0.061*	0.876 (2)
H20C	0.957600	1.076219	0.409194	0.061*	0.876 (2)
C16A	0.97712 (12)	0.59637 (14)	0.43206 (5)	0.0234 (2)	0.124 (2)
H16C	1.062281	0.519706	0.427870	0.028*	0.124 (2)
H16D	0.980364	0.639019	0.471557	0.028*	0.124 (2)
C17A	0.9931 (9)	0.7259 (9)	0.3882 (3)	0.0243 (3)	0.124 (2)
H17C	0.910011	0.803538	0.394727	0.029*	0.124 (2)
H17D	0.977141	0.681752	0.349278	0.029*	0.124 (2)
C18A	1.1499 (8)	0.8083 (8)	0.3900 (4)	0.0253 (3)	0.124 (2)
H18C	1.232160	0.730682	0.398215	0.030*	0.124 (2)
H18D	1.170922	0.853276	0.351630	0.030*	0.124 (2)
C19A	1.1596 (11)	0.9373 (10)	0.4346 (4)	0.0315 (3)	0.124 (2)
H19C	1.269877	0.952670	0.445714	0.038*	0.124 (2)
H19D	1.102479	0.904136	0.469368	0.038*	0.124 (2)
C20A	1.093 (3)	1.0922 (12)	0.4137 (10)	0.0403 (5)	0.124 (2)
H20D	1.150894	1.127650	0.380078	0.061*	0.124 (2)
H20E	1.101665	1.169795	0.444423	0.061*	0.124 (2)
H20F	0.983034	1.078467	0.403273	0.061*	0.124 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0187 (4)	0.0286 (4)	0.0199 (4)	−0.0031 (3)	0.0018 (3)	−0.0075 (3)
O2	0.0168 (4)	0.0281 (4)	0.0230 (4)	−0.0014 (3)	0.0074 (3)	−0.0041 (3)
N1	0.0139 (4)	0.0234 (5)	0.0169 (4)	−0.0037 (3)	0.0042 (3)	−0.0052 (3)
N2	0.0128 (4)	0.0208 (4)	0.0200 (4)	−0.0026 (3)	0.0029 (3)	−0.0030 (3)
C1	0.0139 (4)	0.0180 (5)	0.0185 (5)	−0.0003 (3)	0.0019 (4)	−0.0014 (4)
C2	0.0137 (4)	0.0185 (5)	0.0151 (5)	−0.0021 (3)	0.0040 (3)	−0.0031 (4)
C3	0.0143 (4)	0.0174 (5)	0.0193 (5)	−0.0008 (3)	0.0025 (4)	−0.0003 (4)
C4	0.0130 (4)	0.0183 (5)	0.0200 (5)	−0.0009 (3)	0.0022 (4)	−0.0004 (4)
C5	0.0190 (5)	0.0241 (5)	0.0206 (5)	−0.0010 (4)	0.0003 (4)	0.0015 (4)
C6	0.0241 (6)	0.0240 (6)	0.0280 (6)	0.0011 (4)	0.0023 (4)	0.0068 (4)
C7	0.0242 (6)	0.0187 (5)	0.0357 (7)	0.0021 (4)	0.0032 (5)	0.0005 (4)
C8	0.0289 (6)	0.0207 (6)	0.0276 (6)	0.0021 (4)	0.0019 (5)	−0.0054 (4)
C9	0.0239 (5)	0.0204 (5)	0.0203 (5)	0.0008 (4)	0.0022 (4)	−0.0017 (4)
C10	0.0166 (5)	0.0150 (5)	0.0165 (5)	−0.0013 (3)	0.0015 (4)	−0.0028 (4)
C11	0.0168 (5)	0.0245 (5)	0.0226 (5)	−0.0016 (4)	0.0036 (4)	0.0017 (4)
C12	0.0171 (5)	0.0312 (6)	0.0277 (6)	0.0009 (4)	0.0009 (4)	0.0002 (5)
C13	0.0260 (6)	0.0285 (6)	0.0278 (6)	0.0014 (4)	−0.0043 (5)	0.0039 (5)

C14	0.0286 (6)	0.0311 (6)	0.0249 (6)	−0.0077 (5)	−0.0008 (5)	0.0086 (5)
C15	0.0186 (5)	0.0271 (6)	0.0230 (6)	−0.0059 (4)	0.0029 (4)	0.0018 (4)
C16	0.0137 (5)	0.0272 (6)	0.0293 (6)	−0.0034 (4)	0.0004 (4)	−0.0044 (5)
C17	0.0178 (5)	0.0221 (6)	0.0330 (8)	−0.0044 (5)	−0.0019 (5)	−0.0039 (6)
C18	0.0157 (5)	0.0267 (7)	0.0334 (8)	−0.0048 (5)	−0.0028 (5)	−0.0018 (6)
C19	0.0198 (6)	0.0308 (7)	0.0440 (9)	−0.0077 (5)	0.0029 (6)	0.0045 (6)
C20	0.0269 (13)	0.0265 (7)	0.0677 (13)	−0.0030 (6)	0.0068 (9)	−0.0033 (8)
C16A	0.0137 (5)	0.0272 (6)	0.0293 (6)	−0.0034 (4)	0.0004 (4)	−0.0044 (5)
C17A	0.0178 (5)	0.0221 (6)	0.0330 (8)	−0.0044 (5)	−0.0019 (5)	−0.0039 (6)
C18A	0.0157 (5)	0.0267 (7)	0.0334 (8)	−0.0048 (5)	−0.0028 (5)	−0.0018 (6)
C19A	0.0198 (6)	0.0308 (7)	0.0440 (9)	−0.0077 (5)	0.0029 (6)	0.0045 (6)
C20A	0.0269 (13)	0.0265 (7)	0.0677 (13)	−0.0030 (6)	0.0068 (9)	−0.0033 (8)

Geometric parameters (Å, º)

O1—C1	1.2238 (13)	C14—H14	0.9500
O2—C3	1.2098 (13)	C15—H15	0.9500
N1—C1	1.3447 (13)	C16—C17	1.5088 (18)
N1—C2	1.4608 (13)	C16—H16A	0.9900
N1—H1	0.884 (16)	C16—H16B	0.9900
N2—C3	1.3732 (14)	C17—C18	1.5250 (17)
N2—C1	1.4062 (13)	C17—H17A	0.9900
N2—C16A	1.4690 (13)	C17—H17B	0.9900
N2—C16	1.4690 (13)	C18—C19	1.523 (2)
C2—C4	1.5305 (15)	C18—H18A	0.9900
C2—C10	1.5316 (15)	C18—H18B	0.9900
C2—C3	1.5455 (14)	C19—C20	1.529 (2)
C4—C5	1.3904 (15)	C19—H19A	0.9900
C4—C9	1.3953 (15)	C19—H19B	0.9900
C5—C6	1.3940 (17)	C20—H20A	0.9800
C5—H5	0.9500	C20—H20B	0.9800
C6—C7	1.3839 (18)	C20—H20C	0.9800
C6—H6	0.9500	C16A—C17A	1.518 (3)
C7—C8	1.3898 (18)	C16A—H16C	0.9900
C7—H7	0.9500	C16A—H16D	0.9900
C8—C9	1.3913 (16)	C17A—C18A	1.523 (3)
C8—H8	0.9500	C17A—H17C	0.9900
C9—H9	0.9500	C17A—H17D	0.9900
C10—C15	1.3899 (15)	C18A—C19A	1.521 (4)
C10—C11	1.3964 (14)	C18A—H18C	0.9900
C11—C12	1.3894 (16)	C18A—H18D	0.9900
C11—H11	0.9500	C19A—C20A	1.528 (4)
C12—C13	1.3859 (18)	C19A—H19C	0.9900
C12—H12	0.9500	C19A—H19D	0.9900
C13—C14	1.3868 (17)	C20A—H20D	0.9800
C13—H13	0.9500	C20A—H20E	0.9800
C14—C15	1.3920 (17)	C20A—H20F	0.9800

C1—N1—C2	113.42 (8)	N2—C16—H16B	108.6
C1—N1—H1	121.5 (10)	C17—C16—H16B	108.6
C2—N1—H1	125.0 (10)	H16A—C16—H16B	107.6
C3—N2—C1	111.38 (8)	C16—C17—C18	110.94 (11)
C3—N2—C16	125.03 (9)	C16—C17—H17A	109.5
C1—N2—C16	123.58 (9)	C18—C17—H17A	109.5
O1—C1—N1	128.08 (10)	C16—C17—H17B	109.5
O1—C1—N2	124.36 (9)	C18—C17—H17B	109.5
N1—C1—N2	107.56 (9)	H17A—C17—H17B	108.0
N1—C2—C4	112.04 (9)	C19—C18—C17	112.90 (11)
N1—C2—C10	109.58 (8)	C19—C18—H18A	109.0
C4—C2—C10	112.09 (8)	C17—C18—H18A	109.0
N1—C2—C3	100.53 (8)	C19—C18—H18B	109.0
C4—C2—C3	109.64 (8)	C17—C18—H18B	109.0
C10—C2—C3	112.43 (8)	H18A—C18—H18B	107.8
O2—C3—N2	126.02 (10)	C18—C19—C20	113.19 (15)
O2—C3—C2	126.90 (10)	C18—C19—H19A	108.9
N2—C3—C2	107.07 (8)	C20—C19—H19A	108.9
C5—C4—C9	119.41 (10)	C18—C19—H19B	108.9
C5—C4—C2	121.00 (10)	C20—C19—H19B	108.9
C9—C4—C2	119.59 (9)	H19A—C19—H19B	107.8
C4—C5—C6	120.20 (11)	C19—C20—H20A	109.5
C4—C5—H5	119.9	C19—C20—H20B	109.5
C6—C5—H5	119.9	H20A—C20—H20B	109.5
C7—C6—C5	120.12 (11)	C19—C20—H20C	109.5
C7—C6—H6	119.9	H20A—C20—H20C	109.5
C5—C6—H6	119.9	H20B—C20—H20C	109.5
C6—C7—C8	120.07 (11)	N2—C16A—C17A	105.8 (3)
C6—C7—H7	120.0	N2—C16A—H16C	110.6
C8—C7—H7	120.0	C17A—C16A—H16C	110.6
C7—C8—C9	119.90 (11)	N2—C16A—H16D	110.6
C7—C8—H8	120.1	C17A—C16A—H16D	110.6
C9—C8—H8	120.1	H16C—C16A—H16D	108.7
C8—C9—C4	120.29 (11)	C16A—C17A—C18A	114.0 (4)
C8—C9—H9	119.9	C16A—C17A—H17C	108.8
C4—C9—H9	119.9	C18A—C17A—H17C	108.8
C15—C10—C11	119.04 (10)	C16A—C17A—H17D	108.8
C15—C10—C2	123.47 (9)	C18A—C17A—H17D	108.8
C11—C10—C2	117.46 (9)	H17C—C17A—H17D	107.7
C12—C11—C10	120.69 (10)	C19A—C18A—C17A	113.7 (4)
C12—C11—H11	119.7	C19A—C18A—H18C	108.8
C10—C11—H11	119.7	C17A—C18A—H18C	108.8
C13—C12—C11	119.86 (11)	C19A—C18A—H18D	108.8
C13—C12—H12	120.1	C17A—C18A—H18D	108.8
C11—C12—H12	120.1	H18C—C18A—H18D	107.7
C12—C13—C14	119.83 (11)	C18A—C19A—C20A	113.5 (5)
C12—C13—H13	120.1	C18A—C19A—H19C	108.9
C14—C13—H13	120.1	C20A—C19A—H19C	108.9

C13—C14—C15	120.39 (11)	C18A—C19A—H19D	108.9
C13—C14—H14	119.8	C20A—C19A—H19D	108.9
C15—C14—H14	119.8	H19C—C19A—H19D	107.7
C10—C15—C14	120.17 (10)	C19A—C20A—H20D	109.5
C10—C15—H15	119.9	C19A—C20A—H20E	109.5
C14—C15—H15	119.9	H20D—C20A—H20E	109.5
N2—C16—C17	114.61 (10)	C19A—C20A—H20F	109.5
N2—C16—H16A	108.6	H20D—C20A—H20F	109.5
C17—C16—H16A	108.6	H20E—C20A—H20F	109.5

C2—N1—C1—O1	179.44 (11)	C4—C5—C6—C7	−0.15 (17)
C2—N1—C1—N2	−0.74 (12)	C5—C6—C7—C8	1.34 (17)
C3—N2—C1—O1	179.30 (10)	C6—C7—C8—C9	−1.27 (17)
C16A—N2—C1—O1	0.42 (17)	C7—C8—C9—C4	0.01 (17)
C16—N2—C1—O1	0.42 (17)	C5—C4—C9—C8	1.17 (16)
C3—N2—C1—N1	−0.53 (12)	C2—C4—C9—C8	−179.95 (10)
C16A—N2—C1—N1	−179.41 (10)	N1—C2—C10—C15	119.65 (11)
C16—N2—C1—N1	−179.41 (10)	C4—C2—C10—C15	−115.31 (11)
C1—N1—C2—C4	117.89 (10)	C3—C2—C10—C15	8.75 (14)
C1—N1—C2—C10	−117.03 (10)	N1—C2—C10—C11	−58.20 (12)
C1—N1—C2—C3	1.52 (11)	C4—C2—C10—C11	66.84 (12)
C1—N2—C3—O2	−178.01 (11)	C3—C2—C10—C11	−169.10 (9)
C16A—N2—C3—O2	0.85 (18)	C15—C10—C11—C12	−1.22 (17)
C16—N2—C3—O2	0.85 (18)	C2—C10—C11—C12	176.73 (10)
C1—N2—C3—C2	1.48 (12)	C10—C11—C12—C13	−0.02 (18)
C16A—N2—C3—C2	−179.66 (10)	C11—C12—C13—C14	1.11 (19)
C16—N2—C3—C2	−179.66 (10)	C12—C13—C14—C15	−1.0 (2)
N1—C2—C3—O2	177.74 (11)	C11—C10—C15—C14	1.37 (17)
C4—C2—C3—O2	59.60 (14)	C2—C10—C15—C14	−176.45 (10)
C10—C2—C3—O2	−65.80 (14)	C13—C14—C15—C10	−0.29 (19)
N1—C2—C3—N2	−1.74 (11)	C3—N2—C16—C17	83.71 (14)
C4—C2—C3—N2	−119.88 (9)	C1—N2—C16—C17	−97.57 (13)
C10—C2—C3—N2	114.71 (10)	N2—C16—C17—C18	175.78 (10)
N1—C2—C4—C5	−17.72 (13)	C16—C17—C18—C19	−178.55 (12)
C10—C2—C4—C5	−141.40 (10)	C17—C18—C19—C20	65.5 (2)
C3—C2—C4—C5	93.00 (11)	C3—N2—C16A—C17A	67.9 (5)
N1—C2—C4—C9	163.42 (9)	C1—N2—C16A—C17A	−113.4 (5)
C10—C2—C4—C9	39.74 (13)	N2—C16A—C17A—C18A	−175.2 (5)
C3—C2—C4—C9	−85.86 (11)	C16A—C17A—C18A—C19A	−84.2 (9)
C9—C4—C5—C6	−1.10 (16)	C17A—C18A—C19A—C20A	−83.6 (13)
C2—C4—C5—C6	−179.96 (10)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.884 (16)	1.972 (16)	2.8538 (12)	175.9 (15)

C12—H12···O2^{ii}	0.95	2.47	3.3960 (14)	166
C14—H14···O2^{iii}	0.95	2.56	3.4475 (15)	156

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) *x*−1, *y*, *z*; (iii) −*x*+3/2, *y*+1/2, −*z*+1/2.