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2-(6-Oxo-3,4-diphenyl-1,6-dihydropyridazin-1-yl)acetic acid

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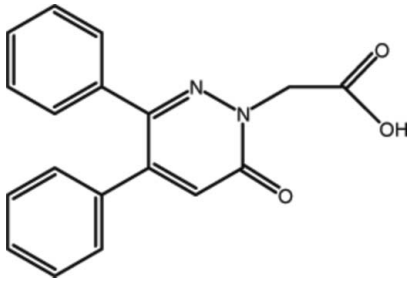
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.055; wR factor = 0.150; data-to-parameter ratio = 17.5.

In the title compound, $C_{18}H_{14}N_2O_3$, the pyridazine ring makes dihedral angles of 72.73 (11) and 49.97 (10)° with the two phenyl rings. The dihedral angle between the two phenyl rings is 52.42 (12)°. The crystal structure is stabilized by intermolecular O—H···O and C—H···O hydrogen-bonding interactions.

Related literature

For related literature, see: Allen *et al.* (1987); Doğruer *et al.* (2007); Moreau *et al.* (1995); Pople & Beveridge (1970); Prout *et al.* (1994).



Experimental

Crystal data

$C_{18}H_{14}N_2O_3$
M_r = 306.31
Monoclinic, $P2_1/c$
a = 10.3646 (11) Å
b = 10.3410 (9) Å
c = 15.5884 (17) Å
β = 109.721 (8)°
V = 1572.8 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 K
0.40 × 0.38 × 0.37 mm

Data collection

Stoe IPDS-2 diffractometer
Absorption correction: none
21463 measured reflections
3658 independent reflections
2225 reflections with $I > 2\sigma(I)$
R_{int} = 0.101

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.151
S = 1.04
3658 reflections
209 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···O1^{i}	0.82	1.78	2.557 (2)	157
C2—H2···O3^{ii}	0.93	2.59	3.422 (3)	150
C13—H13···O2^{iii}	0.93	2.46	3.220 (3)	138

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

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2323).

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supplementary materials

Acta Cryst. (2007). E**63**, o4522 [**doi:10.1107/S1600536807053172**]

2-(6-Oxo-3,4-diphenyl-1,6-dihydropyridazin-1-yl)acetic acid

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Comment

2-[5,6-Diphenyl-3(2*H*)-pyridazinone-2-yl]acetic acid was used as starting material to synthesize 2-[5,6-Diphenyl-3(2*H*)-pyridazinone-2-yl]acetamide derivatives with analgesic and anti-Inflammatory effects. This compound was synthesized for first time by (Doğruer *et al.*, 2007).

All bond lengths and angles in the title compound (I) (Fig. 1) are normal (Allen *et al.*, 1987). The bond lengths for C2═C3, 1.359 (3) Å, C4═N2, 1.306 (3) Å, N1—N2, 1.359 (2) Å and C1═O1, 1.251 (2) Å are comparable with published values for other pyridazinones (Moreau *et al.*, 1995; Prout *et al.*, 1994). In (I), the pyridazine ring (C1–C4/N1/N2) makes dihedral angles of 72.73 (11)° and 49.97 (10)° with two phenyl rings (C5–C10) and (C11—C16), respectively. The dihedral angle between two phenyl rings is 52.42 (12)°.

The quantum-chemical calculation, using the *CNDO* (Pople *et al.*, 1970) aproximation showed that the charges at atoms C1, C4, C18, N1, N2, O1, O2 and O3 are 0.331, 0.109, 0.403, −0.127, −0.094, −0.367, −0.312 and −0.268 e^{-}, respectively. The spatial view of the calculated molecule is shown in Fig. 2. The *HOMO* and *LUMO* energy levels are −10.4162 and 0.8511 eV, respectively. The calculated molecule dipole moment of (I) is 3.795 Debye (1 D = 3.33564 × 10–30 *Cm*). Due to the lack of the strong intermolecular interactions in the crystal structure of (I), the theoretical *CNDO* and experimental X-rays values of the geometric parameters in (I) are almost comparable within the experimental error interval.

The crystal structure of (I) is stabilized by intermolecular O—H···O and C—H···O hydrogen bonding interactions (Table 1, Fig. 3).

Experimental

0.01 mol of ethyl 2-[5,6-Diphenyl-3(2*H*)-pyridazinone-2-yl]acetate in 100 ml 10% NaOH was hydrolyzed for 4 h. After cooling to 278 K, the reaction mixture was acidified 20% HCl. The precipitate was filtered, washed with water to neutral pH and dried and crystallized from 2-propanol (m.p. 491 K, yield 80%), IR ν_{max}(cm^{-1}) (KBr): 3100–2100 (OH), 1725 (CO acid), 1627 (CO amide) (Doğruer *et al.*, 2007).

Refinement

H atoms were positioned geometrically with C–H = 0.93–0.97Å and O—H = 0.82 Å, and constrained to ride on their parent atoms with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(O).

Figures

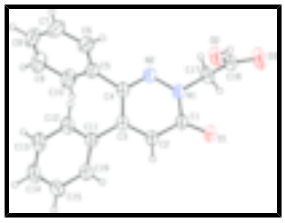


Fig. 1. *ORTEP-3* drawings of the title compound with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level.

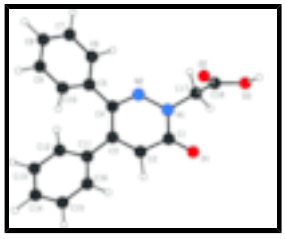


Fig. 2. The spatial view of the title molecule calculated by the *CNDO* approximation.

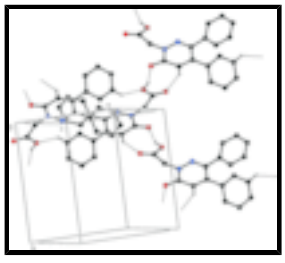


Fig. 3. View of the hydrogen bonding interactions (dash lines) of the title compound in the unit cell. H atoms not involved in hydrogen bonding interactions have been omitted for clarity.

2-(6-Oxo-3,4-diphenyl-1,6-dihydropyridazin-1-yl)acetic acid

Crystal data

$C_{18}H_{14}N_2O_3$	F_{000} = 640
M_r = 306.31	D_x = 1.294 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 37146 reflections
a = 10.3646 (11) Å	θ = 2.0–28.0º
b = 10.3410 (9) Å	μ = 0.09 mm^{-1}
c = 15.5884 (17) Å	T = 296 K
β = 109.721 (8)º	Prism, colourless
V = 1572.8 (3) Å^3	0.40 × 0.38 × 0.37 mm
Z = 4	

Data collection

Stoe IPDS-2 diffractometer	2225 reflections with $I > 2\sigma(I)$
Monochromator: plane graphite	R_{int} = 0.101
Detector resolution: 6.67 pixels mm^{-1}	θ_{max} = 27.8º
T = 296 K	θ_{min} = 2.1º
ω scans	h = −13→13

Absorption correction: none
21463 measured reflections
3658 independent reflections

$k = -13 \rightarrow 13$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.151$
$S = 1.04$
3658 reflections
209 parameters
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
$w = 1/[\sigma^2(F_o^2) + (0.0634P)^2 + 0.0964P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ e Å^{-3}
Extinction correction: SHELXL97 (Sheldrick, 1997), $FC^*=KFC[1+0.001XFC^2\Lambda^3/SIN(2\Theta)]^{-1/4}$
Extinction coefficient: 0.013 (2)

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating –*R*-factor-obs *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and *R*-factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.94042 (12)	0.14434 (14)	0.76943 (10)	0.0709 (5)
O2	0.92925 (14)	−0.17253 (16)	0.77544 (10)	0.0781 (5)
O3	1.08356 (16)	−0.13826 (18)	0.91244 (11)	0.0929 (6)
N1	0.77229 (14)	0.02608 (16)	0.79118 (11)	0.0570 (5)
N2	0.64208 (15)	−0.01944 (16)	0.76872 (11)	0.0599 (5)
C1	0.81545 (17)	0.11781 (19)	0.74420 (13)	0.0575 (6)
C2	0.71116 (18)	0.17567 (19)	0.66976 (13)	0.0590 (6)
C3	0.57856 (17)	0.13681 (18)	0.64688 (12)	0.0533 (6)
C4	0.54875 (17)	0.03339 (19)	0.69902 (13)	0.0544 (6)
C5	0.40883 (18)	−0.0228 (2)	0.67529 (14)	0.0606 (7)
C6	0.3823 (2)	−0.1430 (2)	0.63435 (16)	0.0743 (8)
C7	0.2494 (3)	−0.1894 (3)	0.60170 (19)	0.0942 (10)
C8	0.1447 (3)	−0.1187 (4)	0.6128 (2)	0.1068 (13)

C9	0.1710 (2)	−0.0024 (4)	0.6561 (2)	0.1076 (15)
C10	0.3029 (2)	0.0472 (3)	0.68677 (19)	0.0836 (9)
C11	0.46957 (17)	0.20112 (19)	0.57093 (13)	0.0545 (6)
C12	0.37528 (19)	0.1305 (2)	0.50165 (13)	0.0658 (7)
C13	0.2768 (2)	0.1926 (3)	0.43160 (16)	0.0779 (9)
C14	0.2698 (2)	0.3255 (3)	0.42961 (17)	0.0814 (9)
C15	0.3612 (2)	0.3964 (2)	0.49734 (17)	0.0764 (8)
C16	0.46225 (19)	0.3345 (2)	0.56787 (15)	0.0657 (7)
C17	0.8709 (2)	−0.0297 (2)	0.87331 (14)	0.0654 (7)
C18	0.97349 (19)	−0.1186 (2)	0.85540 (14)	0.0619 (7)
H2	0.73400	0.24090	0.63640	0.0710*
H2A	0.98900	−0.21990	0.76920	0.1170*
H6	0.45380	−0.19270	0.62870	0.0890*
H7	0.23120	−0.26890	0.57210	0.1130*
H8	0.05540	−0.15010	0.59070	0.1280*
H9	0.09990	0.04410	0.66520	0.1290*
H10	0.31980	0.12760	0.71500	0.1000*
H12	0.37890	0.04060	0.50280	0.0790*
H13	0.21480	0.14460	0.38540	0.0940*
H14	0.20290	0.36710	0.38230	0.0980*
H15	0.35570	0.48620	0.49620	0.0920*
H16	0.52510	0.38310	0.61310	0.0790*
H17A	0.82130	−0.07720	0.90590	0.0790*
H17B	0.91970	0.04000	0.91250	0.0790*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0406 (7)	0.0780 (9)	0.0799 (10)	−0.0027 (6)	0.0016 (6)	0.0080 (7)
O2	0.0593 (8)	0.0896 (11)	0.0671 (9)	0.0188 (7)	−0.0026 (7)	−0.0126 (8)
O3	0.0646 (9)	0.1135 (13)	0.0735 (10)	0.0284 (9)	−0.0123 (8)	−0.0078 (9)
N1	0.0416 (7)	0.0679 (10)	0.0542 (9)	0.0041 (6)	0.0065 (7)	0.0057 (7)
N2	0.0473 (8)	0.0704 (10)	0.0580 (9)	0.0011 (7)	0.0124 (7)	0.0059 (8)
C1	0.0432 (9)	0.0610 (11)	0.0609 (11)	0.0004 (8)	0.0078 (8)	−0.0009 (9)
C2	0.0450 (9)	0.0654 (12)	0.0595 (11)	−0.0005 (8)	0.0083 (9)	0.0074 (9)
C3	0.0427 (9)	0.0615 (11)	0.0513 (10)	0.0020 (7)	0.0102 (8)	−0.0003 (8)
C4	0.0430 (9)	0.0651 (12)	0.0515 (10)	0.0026 (7)	0.0111 (8)	0.0013 (8)
C5	0.0475 (10)	0.0738 (13)	0.0567 (11)	−0.0050 (9)	0.0126 (9)	0.0052 (9)
C6	0.0679 (13)	0.0788 (15)	0.0744 (14)	−0.0130 (11)	0.0218 (11)	0.0034 (12)
C7	0.0831 (17)	0.1003 (19)	0.0899 (18)	−0.0398 (15)	0.0171 (15)	0.0045 (15)
C8	0.0551 (14)	0.134 (3)	0.118 (2)	−0.0281 (16)	0.0119 (15)	0.027 (2)
C9	0.0529 (13)	0.129 (3)	0.144 (3)	−0.0006 (15)	0.0375 (16)	0.013 (2)
C10	0.0563 (12)	0.0979 (18)	0.0993 (18)	−0.0012 (11)	0.0300 (13)	−0.0025 (14)
C11	0.0402 (8)	0.0671 (12)	0.0531 (10)	0.0029 (8)	0.0117 (8)	0.0041 (9)
C12	0.0498 (10)	0.0822 (14)	0.0553 (11)	0.0011 (9)	0.0046 (9)	0.0010 (10)
C13	0.0549 (11)	0.1049 (19)	0.0602 (13)	0.0027 (11)	0.0013 (10)	0.0049 (12)
C14	0.0530 (11)	0.113 (2)	0.0688 (14)	0.0168 (12)	0.0081 (11)	0.0239 (14)
C15	0.0608 (12)	0.0790 (15)	0.0858 (16)	0.0142 (10)	0.0199 (12)	0.0218 (12)

C16	0.0504 (10)	0.0720 (13)	0.0681 (13)	0.0019 (9)	0.0113 (10)	0.0069 (10)
C17	0.0551 (11)	0.0790 (14)	0.0524 (11)	0.0101 (9)	0.0053 (9)	0.0082 (10)
C18	0.0489 (10)	0.0696 (13)	0.0565 (11)	0.0043 (9)	0.0037 (9)	0.0053 (9)

Geometric parameters (Å, °)

O1—C1	1.251 (2)	C11—C12	1.394 (3)
O2—C18	1.300 (3)	C12—C13	1.376 (3)
O3—C18	1.204 (3)	C13—C14	1.376 (4)
O2—H2A	0.8200	C14—C15	1.369 (4)
N1—C1	1.363 (3)	C15—C16	1.392 (3)
N1—C17	1.461 (3)	C17—C18	1.501 (3)
N1—N2	1.359 (2)	C2—H2	0.9300
N2—C4	1.306 (3)	C6—H6	0.9300
C1—C2	1.424 (3)	C7—H7	0.9300
C2—C3	1.359 (3)	C8—H8	0.9300
C3—C4	1.439 (3)	C9—H9	0.9300
C3—C11	1.489 (3)	C10—H10	0.9300
C4—C5	1.489 (3)	C12—H12	0.9300
C5—C10	1.376 (3)	C13—H13	0.9300
C5—C6	1.382 (3)	C14—H14	0.9300
C6—C7	1.383 (4)	C15—H15	0.9300
C7—C8	1.367 (5)	C16—H16	0.9300
C8—C9	1.361 (6)	C17—H17A	0.9700
C9—C10	1.386 (4)	C17—H17B	0.9700
C11—C16	1.381 (3)		
O1···C18	3.000 (3)	C12···C10	3.331 (3)
O1···C8^{i}	3.354 (4)	C13···O2^{iv}	3.220 (3)
O1···O2^{ii}	2.557 (2)	C15···C15^{x}	3.566 (3)
O2···O1^{iii}	2.557 (2)	C16···N2^{i}	3.435 (3)
O2···C1	3.202 (3)	C18···O1	3.000 (3)
O2···N1	2.682 (2)	C1···H2A^{ii}	2.6900
O2···C13^{iv}	3.220 (3)	C2···H16	2.8200
O3···C7^{v}	3.378 (3)	C4···H12	2.9700
O1···H2A^{ii}	1.7800	C5···H12	2.6800
O1···H9^{vi}	2.8700	C6···H12	2.7900
O1···H17B	2.5500	C15···H17A^{i}	2.8000
O1···H14^{vii}	2.7000	C16···H15^{x}	3.0400
O2···H13^{iv}	2.4600	C16···H2	2.8200
O3···H2^{iii}	2.5900	H2···C16	2.8200
O3···H7^{v}	2.6200	H2···H16	2.5400
N1···O2	2.682 (2)	H2···O3^{ii}	2.5900
N1···C7^{i}	3.428 (3)	H2A···O1^{iii}	1.7800
N2···C16^{viii}	3.435 (3)	H2A···C1^{iii}	2.6900
C1···O2	3.202 (3)	H7···H17B^{viii}	2.5800

C1···C7^{i}	3.360 (4)	H7···O3^{ix}	2.6200
C1···C8^{i}	3.456 (4)	H9···O1^{xi}	2.8700
C5···C12	3.054 (3)	H12···C4	2.9700
C6···C12	3.490 (3)	H12···C5	2.6800
C7···C1^{viii}	3.360 (4)	H12···C6	2.7900
C7···N1^{viii}	3.428 (3)	H13···O2^{iv}	2.4600
C7···O3^{ix}	3.378 (3)	H14···O1^{xii}	2.7000
C8···C1^{viii}	3.456 (4)	H15···C16^{x}	3.0400
C8···O1^{viii}	3.354 (4)	H16···C2	2.8200
C10···C12	3.331 (3)	H16···H2	2.5400
C10···C11	3.299 (3)	H17A···C15^{viii}	2.8000
C11···C10	3.299 (3)	H17B···O1	2.5500
C12···C6	3.490 (3)	H17B···H7^{i}	2.5800
C12···C5	3.054 (3)		
C18—O2—H2A	109.00	N1—C17—C18	114.13 (17)
N2—N1—C17	115.43 (16)	O2—C18—C17	113.47 (18)
C1—N1—C17	119.11 (16)	O3—C18—C17	121.35 (19)
N2—N1—C1	125.46 (16)	O2—C18—O3	125.2 (2)
N1—N2—C4	117.51 (16)	C1—C2—H2	120.00
O1—C1—C2	125.81 (18)	C3—C2—H2	120.00
N1—C1—C2	115.72 (17)	C5—C6—H6	120.00
O1—C1—N1	118.47 (17)	C7—C6—H6	120.00
C1—C2—C3	120.81 (18)	C6—C7—H7	120.00
C2—C3—C4	117.55 (17)	C8—C7—H7	120.00
C4—C3—C11	122.09 (17)	C7—C8—H8	120.00
C2—C3—C11	120.35 (17)	C9—C8—H8	120.00
N2—C4—C3	122.76 (17)	C8—C9—H9	120.00
C3—C4—C5	121.79 (17)	C10—C9—H9	120.00
N2—C4—C5	115.44 (17)	C5—C10—H10	120.00
C4—C5—C6	119.42 (18)	C9—C10—H10	120.00
C4—C5—C10	121.0 (2)	C11—C12—H12	120.00
C6—C5—C10	119.3 (2)	C13—C12—H12	120.00
C5—C6—C7	120.0 (2)	C12—C13—H13	120.00
C6—C7—C8	120.2 (3)	C14—C13—H13	120.00
C7—C8—C9	120.1 (3)	C13—C14—H14	120.00
C8—C9—C10	120.5 (3)	C15—C14—H14	120.00
C5—C10—C9	119.9 (3)	C14—C15—H15	120.00
C3—C11—C12	121.84 (18)	C16—C15—H15	120.00
C3—C11—C16	119.44 (18)	C11—C16—H16	120.00
C12—C11—C16	118.72 (18)	C15—C16—H16	120.00
C11—C12—C13	120.6 (2)	N1—C17—H17A	109.00
C12—C13—C14	120.2 (2)	N1—C17—H17B	109.00
C13—C14—C15	120.0 (2)	C18—C17—H17A	109.00
C14—C15—C16	120.2 (2)	C18—C17—H17B	109.00
C11—C16—C15	120.28 (19)	H17A—C17—H17B	108.00
C1—N1—N2—C4	−3.7 (3)	N2—C4—C5—C10	112.0 (2)
C17—N1—N2—C4	175.89 (17)	N2—C4—C5—C6	−73.2 (3)

N2—N1—C1—O1	−175.38 (17)	C3—C4—C5—C6	105.4 (2)
C17—N1—C1—O1	5.1 (3)	C3—C4—C5—C10	−69.4 (3)
N2—N1—C1—C2	4.9 (3)	C4—C5—C6—C7	−172.0 (2)
C17—N1—C1—C2	−174.62 (17)	C6—C5—C10—C9	−1.0 (4)
N2—N1—C17—C18	109.0 (2)	C4—C5—C10—C9	173.8 (2)
C1—N1—C17—C18	−71.4 (2)	C10—C5—C6—C7	2.9 (4)
N1—N2—C4—C3	−0.6 (3)	C5—C6—C7—C8	−2.4 (4)
N1—N2—C4—C5	178.03 (16)	C6—C7—C8—C9	0.0 (5)
N1—C1—C2—C3	−2.0 (3)	C7—C8—C9—C10	2.0 (5)
O1—C1—C2—C3	178.26 (19)	C8—C9—C10—C5	−1.5 (5)
C1—C2—C3—C4	−1.6 (3)	C3—C11—C12—C13	−179.09 (19)
C1—C2—C3—C11	177.87 (17)	C12—C11—C16—C15	0.8 (3)
C11—C3—C4—C5	5.1 (3)	C16—C11—C12—C13	0.0 (3)
C2—C3—C11—C12	130.3 (2)	C3—C11—C16—C15	179.9 (2)
C4—C3—C11—C12	−50.3 (3)	C11—C12—C13—C14	−0.5 (3)
C4—C3—C11—C16	130.7 (2)	C12—C13—C14—C15	0.2 (3)
C2—C3—C11—C16	−48.7 (3)	C13—C14—C15—C16	0.6 (4)
C11—C3—C4—N2	−176.41 (18)	C14—C15—C16—C11	−1.2 (3)
C2—C3—C4—N2	3.0 (3)	N1—C17—C18—O2	−26.4 (3)
C2—C3—C4—C5	−175.47 (18)	N1—C17—C18—O3	155.6 (2)

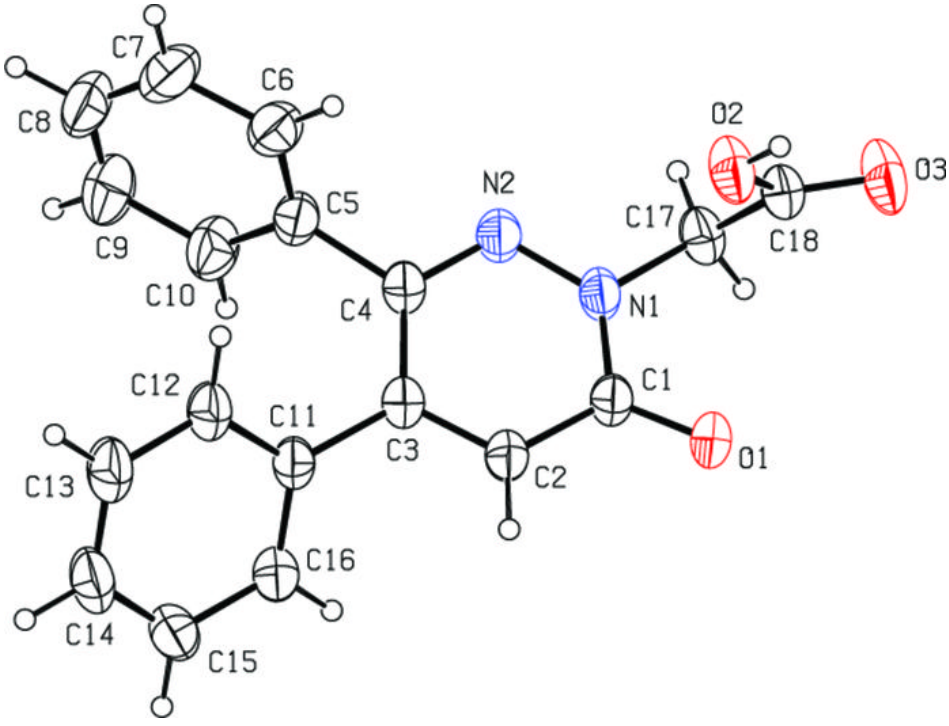
Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+3/2; (ii) −*x*+2, *y*+1/2, −*z*+3/2; (iii) −*x*+2, *y*−1/2, −*z*+3/2; (iv) −*x*+1, −*y*, −*z*+1; (v) *x*+1, −*y*−1/2, *z*+1/2; (vi) *x*+1, *y*, *z*; (vii) *x*+1, −*y*+1/2, *z*+1/2; (viii) −*x*+1, *y*−1/2, −*z*+3/2; (ix) *x*−1, −*y*−1/2, *z*−1/2; (x) −*x*+1, −*y*+1, −*z*+1; (xi) *x*−1, *y*, *z*; (xii) *x*−1, −*y*+1/2, *z*−1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2A···O1^{iii}	0.82	1.78	2.557 (2)	157
C2—H2···O3^{ii}	0.93	2.59	3.422 (3)	150
C13—H13···O2^{iv}	0.93	2.46	3.220 (3)	138

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

Fig. 1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C6
C8
C5
N2
O2
O3
C17
C18
C9
C10
C4
N1
C12
C11
C3
C1
O1
C13
C2
C16
C14
C15

Fig. 2

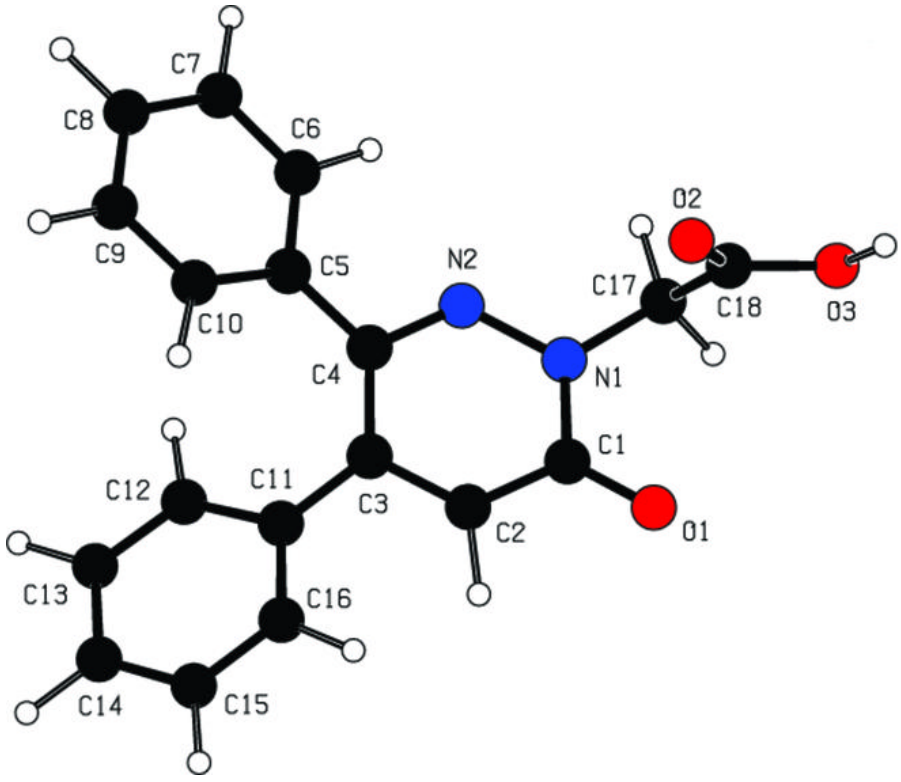
C7
C8
C6
C9
C5
N2
O2
C17
C18
O3
C10
C4
N1
C1
C12
C11
C3
C2
O1
C13
C16
C14
C15

Fig. 3