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1-[(Oxiran-2-yl)methyl]-3-phenyl-1,2-dihydroquinoxalin-2-one

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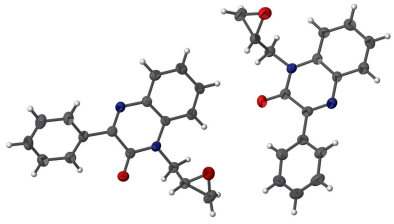
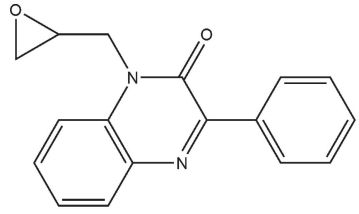
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title compound, $C_{17}H_{14}N_2O_2$, consists of two independent molecules differing mainly in the orientations of the phenyl and oxirane substituents. In the first molecule, the dihedral angle between the dihydroquinoxaline ring system and phenyl ring is 28.4 (2)° and the N—C—C—O torsion angle is 87.8 (5)°; corresponding data for the second molecule are 23.1 (2) and −85.6 (5)°, respectively. In the crystal, offset π-stacking interactions between the dihydroquinoxaline moieties form oblique stacks, which are connected into layers parallel to the *bc* plane by C—H···O hydrogen bonds and C—H···π(ring) interactions. Additional C—H···π(ring) interactions tie the layers together. The model was refined as a two-component twin.

3D view



Chemical scheme



Structure description

In a continuation of our previous work on the synthesis and biological properties of quinoxaline derivatives (Ramli & Essassi, 2015; Abad *et al.*, 2018), we report herein on the preparation and crystal structure of the title compound.

The asymmetric unit (Fig. 1) consists of two independent molecules differing in the orientation of the pendant phenyl and oxirane substituents. Thus the N1—C7—C9—C10 torsion angle is 27.8 (7)° while the N3—C24—C26—C27 angle is −22.8 (7)°. In addition, the C1—N2—C15—C16 torsion angle is −93.7 (5)° while the C18—N4—C32—C33 angle is 94.1 (5)°. The dihydroquinoxalone moieties are virtually planar (r.m.s. deviations for the C1 and C18 molecules = 0.026 and 0.024 Å, respectively) with the largest deviation from the mean plane being the carbonyl carbon atoms C8 [0.038 (5) Å] and C25

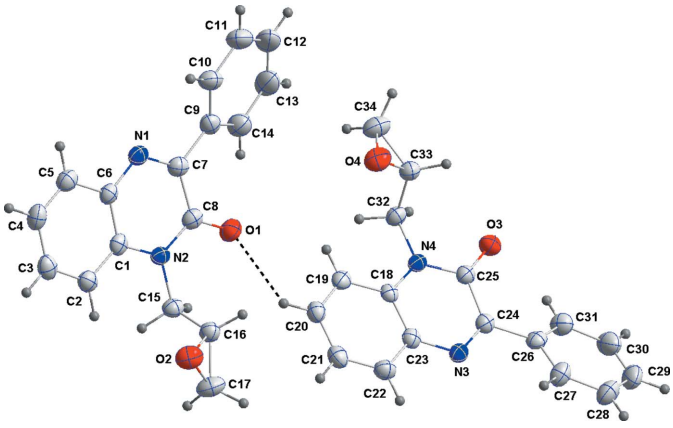


Figure 1
The asymmetric unit with the atom-labeling scheme and 50% probability ellipsoids. The intermolecular C—H···O hydrogen bond is shown by a dashed line

[0.038 (5) Å]. The oxygen atoms O1 and O3 were not included in the mean-plane calculations and lie, respectively, 0.098 (4) and 0.109 (4) Å from the mean planes.

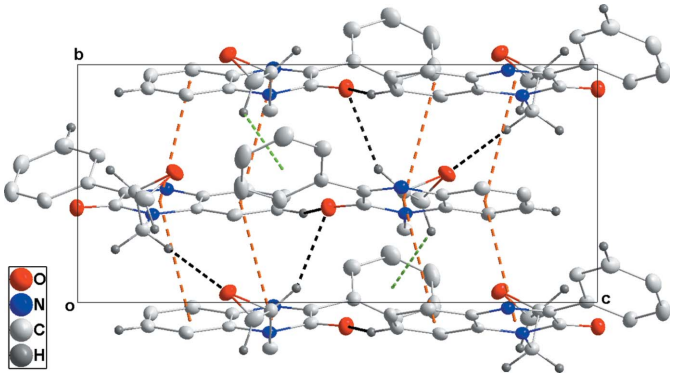


Figure 2
The packing viewed along the *a*-axis direction giving an elevation view of one layer. C—H···O hydrogen bonds and C—H···π(ring) and π-stacking interactions are shown, respectively, by black, green and orange dashed lines.

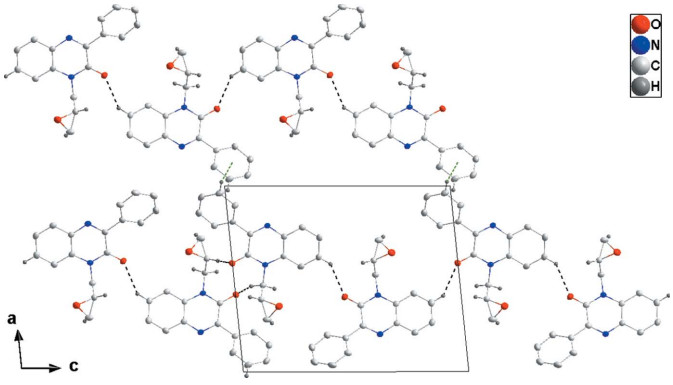


Figure 3
The packing viewed along the *b*-axis direction giving a view of portions of two layers. Intermolecular interactions are depicted as in Fig. 2.

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

*Cg*4 and *Cg*9 are the centroids of the C9–C14 and C26–C31 benzene rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O3^{i}	0.95	2.45	3.263 (7)	143
C16—H16···O1^{ii}	1.00	2.58	3.489 (7)	151
C20—H20···O1	0.95	2.46	3.258 (6)	142
C32—H32*A*···O2^{iii}	0.99	2.55	3.520 (6)	168
C32—H32*B*···O3^{iv}	0.99	2.58	3.465 (6)	149
C33—H33···O3^{v}	1.00	2.59	3.504 (6)	152
C17—H17*A*···*Cg*4^{iii}	0.99	2.91	3.556 (6)	123
C28—H28···*Cg*9^{vi}	0.95	2.62	3.512 (2)	156
C34—H34*B*···*Cg*9^{iv}	0.99	2.93	3.587 (6)	125

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{14}N_2O_2$
M_r	278.30
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	200
a, *b*, *c* (Å)	12.7853 (3), 7.0167 (2), 15.4215 (4)
β (°)	95.718 (1)
V (Å^3)	1376.59 (6)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.72
Crystal size (mm)	0.32 × 0.09 × 0.02
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*TWINABS*; Sheldrick, 2009)
T_{min}, T_{max}	0.80, 0.99
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	17578, 17578, 13057
R_{int}	0.053
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.619
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.062, 0.147, 1.04
No. of reflections	17578
No. of parameters	381
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.20, −0.19
Absolute structure	Flack *x* determined using 1479 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.32 (17)

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

In the crystal, the two independent molecules form oblique stacks along the *b*-axis direction in an alternating head-to-tail fashion through offset π-stacking interactions between the dihydroquinoxalone moieties [centroid–centroid separations = 3.703 (3) and 3.546 (3) Å for the C1/C6/N1/C7/C8/N2 ring and the C18–C25 rings at $(-x+1, y-\frac{1}{2}, -z+1)$ and at $(-x+1, y+\frac{1}{2}, -z+1)$, respectively, and 3.620 (3) and 3.616 (3) Å for the C1–C6 ring and the C18/C23/N3/C24/C25/N4 rings at

($-x+1, y-\frac{1}{2}, -z+1$) and ($-x+1, y+\frac{1}{2}, -z+1$), respectively]. These interactions are accompanied by C—H···O hydrogen bonds as well as C17—H17*A*···*Cg*4 and C34—H34*B*···*Cg*9 C—H···π interactions (Table 1), which reinforce and connect the stacks, forming layers parallel to the *bc* plane (Fig. 2). The layers are weakly connected along the *a*-axis direction by complementary C28—H28···*Cg*9 interactions (Table 1 and Fig. 3).

Synthesis and crystallization

To a solution of 2-oxo-3-phenyl-1,2-dihydroquinoxaline (0.5 g, 2.25 mmol) in dichloromethane (20 ml) were added 2-(chloromethyl)oxirane (0.2 ml, 2.25 mmol), sodium hydroxide (0.1 g, 2.25 mmol) and a catalytic quantity of tetra-*n*-butylammonium bromide. The reaction mixture was stirred at room temperature for 24 h. The solution was filtered and the solvent removed under reduced pressure. The residue thus obtained was chromatographed on a silica gel column using a hexane/ethyl acetate 9:1 mixture as eluent. The solid obtained was recrystallized from ethanol solution to afford colourless plates of the title compound.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The model was refined as a two-component twin.

Funding information

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full crystallographic data

IUCrData (2018). **3**, x180610 [https://doi.org/10.1107/S2414314618006107]

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Crystal data

$C_{17}H_{14}N_2O_2$
M_r = 278.30
Monoclinic, $P2_1$
a = 12.7853 (3) Å
b = 7.0167 (2) Å
c = 15.4215 (4) Å
β = 95.718 (1)°
V = 1376.59 (6) Å^3
Z = 4
$F(000)$ = 584
D_x = 1.343 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9964 reflections
θ = 3.5–72.5°
μ = 0.72 mm^{-1}
T = 200 K
Plate, colourless
0.32 × 0.09 × 0.02 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro-focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*TWINABS*; Sheldrick, 2009)
T_{min} = 0.80, T_{max} = 0.99
17578 measured reflections
17578 independent reflections
13057 reflections with $I > 2\sigma(I)$
R_{int} = 0.053
θ_{max} = 72.5°, θ_{min} = 2.9°
h = −15→15
k = −8→8
l = −16→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.147
S = 1.04
17578 reflections
381 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
$w = 1/[\sigma^2(F_o^2) + (0.0548P)^2 + 0.1212P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Extinction correction: *SHELXL2018* (Sheldrick, 2015*b*), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0029 (8)
Absolute structure: Flack x determined using 1479 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.32 (17)

Special details

Experimental. Analysis of 995 reflections having I/σ(I) > 12 and chosen from the full data set with*CELL_NOW* (Sheldrick, 2008) showed the crystal to belong to the monoclinic system and to be twinned by a 180° rotation about the *c* axis. The raw data were processed using the multi-component version of *SAINT* under control of the two-component orientation file generated by *CELL_NOW*.

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 $F^2 > 2\mathrm{sigma}(F^2)$ 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 - 1.00 Å) and included as riding contributions with isotropic displacement parameters 1.2 - 1.5 times those of the attached atoms. Refined as a 2-component twin.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.4028 (3)	0.3996 (6)	0.4830 (2)	0.0412 (10)
O2	0.6415 (3)	0.5409 (6)	0.7106 (2)	0.0431 (10)
N1	0.2018 (3)	0.4840 (6)	0.6230 (3)	0.0312 (10)
N2	0.4120 (3)	0.3738 (6)	0.6307 (3)	0.0274 (9)
C1	0.3661 (4)	0.3984 (7)	0.7081 (3)	0.0273 (11)
C2	0.4211 (4)	0.3726 (7)	0.7906 (3)	0.0330 (12)
H2	0.493027	0.336082	0.795627	0.040*
C3	0.3705 (4)	0.4005 (8)	0.8644 (4)	0.0367 (13)
H3	0.408232	0.383106	0.920066	0.044*
C4	0.2656 (4)	0.4535 (8)	0.8589 (3)	0.0376 (12)
H4	0.231870	0.471955	0.910437	0.045*
C5	0.2108 (4)	0.4791 (7)	0.7786 (3)	0.0355 (12)
H5	0.138839	0.515034	0.774595	0.043*
C6	0.2607 (4)	0.4525 (7)	0.7020 (3)	0.0280 (10)
C7	0.2469 (4)	0.4674 (7)	0.5511 (3)	0.0300 (11)
C8	0.3583 (4)	0.4127 (7)	0.5506 (3)	0.0302 (11)
C9	0.1817 (4)	0.5144 (7)	0.4689 (3)	0.0330 (12)
C10	0.1001 (4)	0.6458 (8)	0.4718 (4)	0.0404 (13)
H10	0.087995	0.701449	0.526022	0.049*
C11	0.0361 (5)	0.6973 (10)	0.3972 (4)	0.0535 (17)
H11	−0.017817	0.789438	0.400177	0.064*
C12	0.0522 (5)	0.6125 (11)	0.3188 (4)	0.0587 (19)
H12	0.008554	0.645194	0.267447	0.070*
C13	0.1312 (5)	0.4809 (11)	0.3151 (4)	0.0556 (18)
H13	0.140663	0.421709	0.260983	0.067*
C14	0.1974 (4)	0.4325 (9)	0.3886 (4)	0.0438 (14)
H14	0.253044	0.344351	0.384318	0.053*
C15	0.5214 (4)	0.3070 (7)	0.6294 (4)	0.0314 (11)
H15A	0.525781	0.225748	0.577398	0.038*
H15B	0.540449	0.227476	0.681603	0.038*

C16	0.5989 (4)	0.4659 (7)	0.6277 (3)	0.0317 (11)
H16	0.586626	0.559289	0.578804	0.038*
C17	0.7079 (4)	0.4289 (9)	0.6599 (4)	0.0438 (14)
H17A	0.726594	0.298482	0.680493	0.053*
H17B	0.763298	0.496150	0.631421	0.053*
O3	0.5845 (3)	0.3974 (6)	−0.0013 (2)	0.0383 (9)
O4	0.3526 (3)	0.5469 (6)	0.1877 (2)	0.0439 (10)
N3	0.7867 (3)	0.4763 (6)	0.1718 (3)	0.0286 (9)
N4	0.5762 (3)	0.3701 (6)	0.1442 (3)	0.0262 (9)
C18	0.6218 (4)	0.3933 (7)	0.2297 (3)	0.0239 (10)
C19	0.5665 (4)	0.3672 (7)	0.3026 (3)	0.0310 (11)
H19	0.494428	0.331880	0.295367	0.037*
C20	0.6173 (4)	0.3931 (7)	0.3853 (3)	0.0313 (11)
H20	0.579565	0.374620	0.434718	0.038*
C21	0.7226 (4)	0.4457 (8)	0.3972 (3)	0.0362 (12)
H21	0.756429	0.463735	0.454327	0.043*
C22	0.7776 (4)	0.4715 (7)	0.3258 (3)	0.0337 (12)
H22	0.849695	0.506572	0.333827	0.040*
C23	0.7282 (4)	0.4465 (7)	0.2412 (3)	0.0273 (10)
C24	0.7419 (4)	0.4606 (7)	0.0924 (3)	0.0275 (10)
C25	0.6298 (4)	0.4082 (7)	0.0731 (3)	0.0274 (11)
C26	0.8073 (4)	0.5017 (7)	0.0204 (3)	0.0295 (11)
C27	0.8958 (4)	0.6170 (7)	0.0383 (4)	0.0367 (12)
H27	0.910857	0.669315	0.094984	0.044*
C28	0.9622 (5)	0.6563 (9)	−0.0252 (4)	0.0454 (14)
H28	1.022013	0.735342	−0.012094	0.054*
C29	0.9411 (5)	0.5801 (9)	−0.1077 (4)	0.0473 (15)
H29	0.986184	0.607713	−0.151485	0.057*
C30	0.8555 (4)	0.4651 (10)	−0.1264 (4)	0.0487 (15)
H30	0.842563	0.410186	−0.182770	0.058*
C31	0.7869 (4)	0.4276 (8)	−0.0634 (3)	0.0378 (12)
H31	0.726240	0.351452	−0.077786	0.045*
C32	0.4665 (4)	0.3043 (7)	0.1257 (3)	0.0300 (11)
H32A	0.447343	0.225915	0.175054	0.036*
H32B	0.461079	0.222681	0.073054	0.036*
C33	0.3905 (4)	0.4656 (7)	0.1115 (3)	0.0310 (11)
H33	0.402167	0.555837	0.063156	0.037*
C34	0.2818 (4)	0.4357 (9)	0.1292 (4)	0.0464 (14)
H34A	0.226085	0.504144	0.092328	0.056*
H34B	0.261803	0.307448	0.148635	0.056*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.036 (2)	0.053 (3)	0.036 (2)	0.0029 (18)	0.0109 (16)	−0.0019 (18)
O2	0.041 (2)	0.042 (2)	0.046 (2)	−0.0012 (17)	0.0010 (17)	−0.0139 (18)
N1	0.028 (2)	0.030 (2)	0.036 (3)	−0.0024 (17)	0.0041 (17)	0.0001 (19)
N2	0.025 (2)	0.024 (2)	0.033 (2)	0.0000 (16)	0.0021 (16)	0.0001 (18)

C1	0.032 (3)	0.018 (2)	0.033 (3)	−0.0050 (19)	0.006 (2)	−0.001 (2)
C2	0.033 (3)	0.029 (3)	0.036 (3)	−0.004 (2)	0.001 (2)	0.003 (2)
C3	0.045 (3)	0.030 (3)	0.035 (3)	−0.008 (2)	0.003 (2)	0.002 (2)
C4	0.045 (3)	0.037 (3)	0.033 (3)	−0.009 (3)	0.012 (2)	−0.001 (2)
C5	0.034 (3)	0.032 (3)	0.042 (3)	−0.003 (2)	0.008 (2)	0.000 (3)
C6	0.029 (2)	0.023 (2)	0.032 (3)	−0.003 (2)	0.0060 (19)	0.000 (2)
C7	0.029 (3)	0.025 (3)	0.036 (3)	−0.003 (2)	0.000 (2)	−0.002 (2)
C8	0.029 (3)	0.024 (3)	0.037 (3)	−0.003 (2)	0.004 (2)	−0.003 (2)
C9	0.032 (3)	0.033 (3)	0.033 (3)	−0.006 (2)	0.000 (2)	0.000 (2)
C10	0.029 (3)	0.044 (3)	0.048 (3)	0.001 (2)	−0.001 (2)	0.001 (3)
C11	0.031 (3)	0.065 (4)	0.062 (5)	0.002 (3)	−0.004 (3)	0.011 (3)
C12	0.037 (4)	0.091 (6)	0.046 (4)	−0.014 (3)	−0.007 (3)	0.013 (4)
C13	0.046 (4)	0.086 (5)	0.035 (3)	−0.011 (3)	0.000 (2)	−0.003 (3)
C14	0.039 (3)	0.054 (4)	0.038 (3)	−0.003 (3)	0.003 (2)	−0.006 (3)
C15	0.028 (3)	0.027 (3)	0.039 (3)	0.003 (2)	0.003 (2)	0.000 (2)
C16	0.031 (3)	0.033 (3)	0.031 (3)	−0.001 (2)	0.0029 (19)	−0.001 (2)
C17	0.029 (3)	0.045 (3)	0.058 (4)	0.002 (3)	0.004 (2)	−0.011 (3)
O3	0.034 (2)	0.047 (2)	0.033 (2)	−0.0020 (17)	−0.0005 (15)	0.0004 (18)
O4	0.044 (2)	0.043 (2)	0.046 (2)	0.0040 (18)	0.0080 (17)	−0.0128 (18)
N3	0.027 (2)	0.027 (2)	0.031 (2)	−0.0012 (17)	0.0046 (16)	0.0000 (18)
N4	0.023 (2)	0.024 (2)	0.032 (2)	−0.0003 (16)	0.0036 (16)	0.0003 (18)
C18	0.028 (3)	0.017 (2)	0.026 (3)	0.0034 (19)	0.0027 (18)	0.0013 (19)
C19	0.029 (3)	0.025 (3)	0.039 (3)	0.004 (2)	0.007 (2)	0.005 (2)
C20	0.037 (3)	0.029 (3)	0.029 (3)	0.005 (2)	0.008 (2)	0.003 (2)
C21	0.044 (3)	0.034 (3)	0.031 (3)	0.008 (3)	0.004 (2)	0.004 (2)
C22	0.031 (3)	0.031 (3)	0.038 (3)	−0.001 (2)	0.000 (2)	0.000 (2)
C23	0.032 (3)	0.019 (2)	0.031 (3)	0.001 (2)	0.005 (2)	0.001 (2)
C24	0.029 (3)	0.022 (2)	0.032 (3)	0.000 (2)	0.0036 (19)	0.000 (2)
C25	0.028 (2)	0.022 (2)	0.032 (3)	0.0014 (19)	0.004 (2)	0.001 (2)
C26	0.026 (3)	0.027 (3)	0.037 (3)	0.005 (2)	0.006 (2)	0.000 (2)
C27	0.038 (3)	0.033 (3)	0.041 (3)	−0.003 (2)	0.013 (2)	−0.004 (2)
C28	0.038 (3)	0.043 (3)	0.057 (4)	−0.005 (3)	0.016 (3)	0.001 (3)
C29	0.044 (4)	0.059 (4)	0.042 (4)	0.007 (3)	0.019 (3)	0.009 (3)
C30	0.045 (3)	0.067 (4)	0.035 (3)	0.010 (3)	0.007 (2)	−0.001 (3)
C31	0.037 (3)	0.041 (3)	0.035 (3)	0.003 (3)	0.004 (2)	−0.005 (2)
C32	0.027 (3)	0.028 (3)	0.035 (3)	−0.003 (2)	0.004 (2)	−0.002 (2)
C33	0.029 (3)	0.031 (3)	0.033 (3)	0.002 (2)	0.0030 (19)	0.000 (2)
C34	0.031 (3)	0.044 (3)	0.064 (4)	−0.002 (3)	0.004 (2)	−0.005 (3)

Geometric parameters (Å, º)

O1—C8	1.239 (6)	O3—C25	1.235 (6)
O2—C16	1.438 (6)	O4—C33	1.434 (6)
O2—C17	1.443 (6)	O4—C34	1.442 (7)
N1—C7	1.304 (6)	N3—C24	1.304 (6)
N1—C6	1.385 (6)	N3—C23	1.381 (6)
N2—C8	1.380 (6)	N4—C25	1.376 (6)
N2—C1	1.393 (6)	N4—C18	1.397 (6)

N2—C15	1.476 (6)	N4—C32	1.477 (6)
C1—C6	1.394 (7)	C18—C19	1.398 (7)
C1—C2	1.403 (7)	C18—C23	1.405 (6)
C2—C3	1.377 (7)	C19—C20	1.385 (7)
C2—H2	0.9500	C19—H19	0.9500
C3—C4	1.386 (8)	C20—C21	1.391 (7)
C3—H3	0.9500	C20—H20	0.9500
C4—C5	1.373 (7)	C21—C22	1.377 (7)
C4—H4	0.9500	C21—H21	0.9500
C5—C6	1.410 (7)	C22—C23	1.402 (7)
C5—H5	0.9500	C22—H22	0.9500
C7—C8	1.476 (7)	C24—C25	1.481 (6)
C7—C9	1.484 (7)	C24—C26	1.484 (7)
C9—C10	1.397 (7)	C26—C31	1.393 (7)
C9—C14	1.397 (7)	C26—C27	1.397 (7)
C10—C11	1.391 (8)	C27—C28	1.386 (8)
C10—H10	0.9500	C27—H27	0.9500
C11—C12	1.381 (9)	C28—C29	1.381 (8)
C11—H11	0.9500	C28—H28	0.9500
C12—C13	1.374 (10)	C29—C30	1.368 (8)
C12—H12	0.9500	C29—H29	0.9500
C13—C14	1.388 (8)	C30—C31	1.397 (8)
C13—H13	0.9500	C30—H30	0.9500
C14—H14	0.9500	C31—H31	0.9500
C15—C16	1.494 (7)	C32—C33	1.493 (7)
C15—H15A	0.9900	C32—H32A	0.9900
C15—H15B	0.9900	C32—H32B	0.9900
C16—C17	1.455 (7)	C33—C34	1.459 (7)
C16—H16	1.0000	C33—H33	1.0000
C17—H17A	0.9900	C34—H34A	0.9900
C17—H17B	0.9900	C34—H34B	0.9900

C16—O2—C17	60.7 (3)	C33—O4—C34	61.0 (3)
C7—N1—C6	119.1 (4)	C24—N3—C23	119.5 (4)
C8—N2—C1	121.9 (4)	C25—N4—C18	122.3 (4)
C8—N2—C15	116.0 (4)	C25—N4—C32	116.4 (4)
C1—N2—C15	122.2 (4)	C18—N4—C32	121.2 (4)
N2—C1—C6	117.6 (4)	N4—C18—C19	123.1 (4)
N2—C1—C2	123.0 (5)	N4—C18—C23	117.2 (4)
C6—C1—C2	119.4 (5)	C19—C18—C23	119.6 (4)
C3—C2—C1	119.7 (5)	C20—C19—C18	119.7 (5)
C3—C2—H2	120.1	C20—C19—H19	120.2
C1—C2—H2	120.1	C18—C19—H19	120.2
C2—C3—C4	121.3 (5)	C19—C20—C21	121.0 (5)
C2—C3—H3	119.4	C19—C20—H20	119.5
C4—C3—H3	119.4	C21—C20—H20	119.5
C5—C4—C3	119.6 (5)	C22—C21—C20	119.6 (5)
C5—C4—H4	120.2	C22—C21—H21	120.2

C3—C4—H4	120.2	C20—C21—H21	120.2
C4—C5—C6	120.4 (5)	C21—C22—C23	120.6 (5)
C4—C5—H5	119.8	C21—C22—H22	119.7
C6—C5—H5	119.8	C23—C22—H22	119.7
N1—C6—C1	122.7 (4)	N3—C23—C22	118.2 (4)
N1—C6—C5	117.7 (5)	N3—C23—C18	122.4 (4)
C1—C6—C5	119.7 (5)	C22—C23—C18	119.4 (4)
N1—C7—C8	122.4 (4)	N3—C24—C25	122.4 (4)
N1—C7—C9	116.7 (4)	N3—C24—C26	117.3 (4)
C8—C7—C9	120.9 (5)	C25—C24—C26	120.3 (4)
O1—C8—N2	120.6 (4)	O3—C25—N4	120.2 (4)
O1—C8—C7	123.2 (5)	O3—C25—C24	123.9 (4)
N2—C8—C7	116.2 (4)	N4—C25—C24	115.9 (4)
C10—C9—C14	118.2 (5)	C31—C26—C27	118.2 (5)
C10—C9—C7	118.5 (5)	C31—C26—C24	123.7 (5)
C14—C9—C7	123.3 (5)	C27—C26—C24	118.0 (5)
C11—C10—C9	121.7 (6)	C28—C27—C26	121.1 (5)
C11—C10—H10	119.2	C28—C27—H27	119.5
C9—C10—H10	119.2	C26—C27—H27	119.5
C12—C11—C10	119.1 (6)	C29—C28—C27	119.8 (6)
C12—C11—H11	120.5	C29—C28—H28	120.1
C10—C11—H11	120.5	C27—C28—H28	120.1
C13—C12—C11	120.0 (6)	C30—C29—C28	120.1 (5)
C13—C12—H12	120.0	C30—C29—H29	120.0
C11—C12—H12	120.0	C28—C29—H29	120.0
C12—C13—C14	121.4 (6)	C29—C30—C31	120.6 (5)
C12—C13—H13	119.3	C29—C30—H30	119.7
C14—C13—H13	119.3	C31—C30—H30	119.7
C13—C14—C9	119.6 (6)	C26—C31—C30	120.2 (5)
C13—C14—H14	120.2	C26—C31—H31	119.9
C9—C14—H14	120.2	C30—C31—H31	119.9
N2—C15—C16	113.2 (4)	N4—C32—C33	112.5 (4)
N2—C15—H15A	108.9	N4—C32—H32A	109.1
C16—C15—H15A	108.9	C33—C32—H32A	109.1
N2—C15—H15B	108.9	N4—C32—H32B	109.1
C16—C15—H15B	108.9	C33—C32—H32B	109.1
H15A—C15—H15B	107.7	H32A—C32—H32B	107.8
O2—C16—C17	59.8 (3)	O4—C33—C34	59.8 (3)
O2—C16—C15	116.8 (4)	O4—C33—C32	116.7 (4)
C17—C16—C15	118.4 (5)	C34—C33—C32	118.8 (5)
O2—C16—H16	116.6	O4—C33—H33	116.5
C17—C16—H16	116.6	C34—C33—H33	116.5
C15—C16—H16	116.6	C32—C33—H33	116.5
O2—C17—C16	59.5 (3)	O4—C34—C33	59.2 (3)
O2—C17—H17A	117.8	O4—C34—H34A	117.8
C16—C17—H17A	117.8	C33—C34—H34A	117.8
O2—C17—H17B	117.8	O4—C34—H34B	117.8
C16—C17—H17B	117.8	C33—C34—H34B	117.8

H17A—C17—H17B	115.0	H34A—C34—H34B	115.0
C8—N2—C1—C6	4.0 (7)	C25—N4—C18—C19	175.7 (4)
C15—N2—C1—C6	−176.7 (4)	C32—N4—C18—C19	−3.8 (7)
C8—N2—C1—C2	−175.4 (4)	C25—N4—C18—C23	−3.8 (7)
C15—N2—C1—C2	3.8 (7)	C32—N4—C18—C23	176.7 (4)
N2—C1—C2—C3	179.6 (4)	N4—C18—C19—C20	−179.9 (4)
C6—C1—C2—C3	0.2 (7)	C23—C18—C19—C20	−0.3 (7)
C1—C2—C3—C4	0.1 (8)	C18—C19—C20—C21	0.3 (8)
C2—C3—C4—C5	−0.1 (8)	C19—C20—C21—C22	−0.4 (8)
C3—C4—C5—C6	−0.2 (8)	C20—C21—C22—C23	0.4 (8)
C7—N1—C6—C1	−1.8 (7)	C24—N3—C23—C22	−177.6 (4)
C7—N1—C6—C5	177.4 (4)	C24—N3—C23—C18	2.1 (7)
N2—C1—C6—N1	−0.7 (7)	C21—C22—C23—N3	179.3 (5)
C2—C1—C6—N1	178.8 (5)	C21—C22—C23—C18	−0.5 (8)
N2—C1—C6—C5	−180.0 (4)	N4—C18—C23—N3	0.3 (7)
C2—C1—C6—C5	−0.5 (7)	C19—C18—C23—N3	−179.3 (4)
C4—C5—C6—N1	−178.8 (4)	N4—C18—C23—C22	−180.0 (4)
C4—C5—C6—C1	0.5 (8)	C19—C18—C23—C22	0.4 (7)
C6—N1—C7—C8	1.2 (7)	C23—N3—C24—C25	−1.1 (7)
C6—N1—C7—C9	−176.4 (4)	C23—N3—C24—C26	177.6 (4)
C1—N2—C8—O1	176.1 (4)	C18—N4—C25—O3	−175.4 (4)
C15—N2—C8—O1	−3.2 (7)	C32—N4—C25—O3	4.1 (7)
C1—N2—C8—C7	−4.6 (7)	C18—N4—C25—C24	4.7 (7)
C15—N2—C8—C7	176.2 (4)	C32—N4—C25—C24	−175.8 (4)
N1—C7—C8—O1	−178.7 (5)	N3—C24—C25—O3	177.9 (5)
C9—C7—C8—O1	−1.3 (8)	C26—C24—C25—O3	−0.8 (7)
N1—C7—C8—N2	1.9 (7)	N3—C24—C25—N4	−2.2 (7)
C9—C7—C8—N2	179.4 (4)	C26—C24—C25—N4	179.1 (4)
N1—C7—C9—C10	27.8 (7)	N3—C24—C26—C31	155.4 (5)
C8—C7—C9—C10	−149.8 (5)	C25—C24—C26—C31	−25.9 (7)
N1—C7—C9—C14	−151.7 (5)	N3—C24—C26—C27	−22.8 (7)
C8—C7—C9—C14	30.7 (8)	C25—C24—C26—C27	155.9 (5)
C14—C9—C10—C11	−0.8 (8)	C31—C26—C27—C28	−0.3 (8)
C7—C9—C10—C11	179.7 (5)	C24—C26—C27—C28	178.0 (5)
C9—C10—C11—C12	1.7 (9)	C26—C27—C28—C29	−0.2 (9)
C10—C11—C12—C13	−0.7 (10)	C27—C28—C29—C30	−0.5 (9)
C11—C12—C13—C14	−1.2 (10)	C28—C29—C30—C31	1.8 (9)
C12—C13—C14—C9	2.1 (10)	C27—C26—C31—C30	1.6 (8)
C10—C9—C14—C13	−1.1 (9)	C24—C26—C31—C30	−176.6 (5)
C7—C9—C14—C13	178.4 (6)	C29—C30—C31—C26	−2.4 (9)
C8—N2—C15—C16	85.6 (5)	C25—N4—C32—C33	−85.4 (5)
C1—N2—C15—C16	−93.7 (5)	C18—N4—C32—C33	94.1 (5)
C17—O2—C16—C15	108.8 (5)	C34—O4—C33—C32	−109.3 (5)
N2—C15—C16—O2	87.8 (5)	N4—C32—C33—O4	−85.6 (5)
N2—C15—C16—C17	156.3 (4)	N4—C32—C33—C34	−154.1 (5)
C15—C16—C17—O2	−106.2 (5)	C32—C33—C34—O4	105.9 (5)

Hydrogen-bond geometry (Å, º)

Cg4 and Cg9 are the centroids of the C9–C14 and C26–C31 benzene rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O3^{i}	0.95	2.45	3.263 (7)	143
C16—H16···O1^{ii}	1.00	2.58	3.489 (7)	151
C20—H20···O1	0.95	2.46	3.258 (6)	142
C32—H32*A*···O2^{iii}	0.99	2.55	3.520 (6)	168
C32—H32*B*···O3^{iv}	0.99	2.58	3.465 (6)	149
C33—H33···O3^{v}	1.00	2.59	3.504 (6)	152
C17—H17*A*···*Cg*4^{iii}	0.99	2.91	3.556 (6)	123
C28—H28···*Cg*9^{vi}	0.95	2.62	3.512 (2)	156
C34—H34*B*···*Cg*9^{iv}	0.99	2.93	3.587 (6)	125

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