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1-(Prop-2-en-1-yl)-3-[(prop-2-en-1-yl)oxy]quinoxalin-2(1*H*)-one

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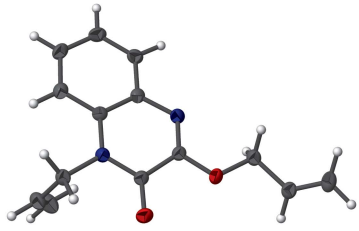
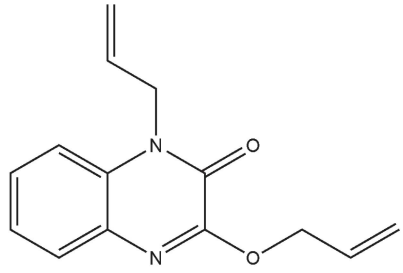
In the title compound, $C_{14}H_{14}N_2O_2$, the dihydroquinoxaline moiety deviates slightly from planarity. In the crystal, zigzag chains are formed by inversion-related C—H···O hydrogen bonds. Adjacent chains are associated through pairwise C—H···π(ring) and π-stacking interactions.

3D view



Chemical scheme



Structure description

Nitrogen-containing heterocyclic compounds are indispensable structural units for medicinal chemists. Among the various heterocyclic compounds, quinoxaline derivatives display important biological activities including anticonvulsant (Ghadage & Shirote, 2011*a*), antitubercular and antimicrobial activities (Ramalingam *et al.*, 2010; Ghadage & Shirote, 2011*b*). They are also used as NMDA receptor antagonists (Lin, 1996). These compounds also have applications in organic synthesis and as ligands in new coordination complexes (Nassar *et al.*, 2013; Attia *et al.*, 2013).

In the title compound (Fig. 1), the C1–C6 ring is planar to within 0.0094 (9) Å (r.m.s. deviation = 0.0065) while the C1/C6/N1/C7/C8/N2 ring deviates by 0.0192 (8) Å from planarity (r.m.s. deviation = 0.0125 Å). The dihedral angle between the mean planes of the two rings is 1.36 (6)°. The N1/C9–C11 unit is planar with an r.m.s. deviation of 0.0041 and subtends an angle of 84.77 (6)° to the dihydroquinoxalinone ring system. The propenyloxy substituent is far from planar, as indicated by the O2—C12—C13—C14 torsion angle of −128.4 (1)°. The plane of the C12–C14 segment subtends an angle of 51.00 (9)° to the dihydroquinoxalinone ring system.

In the crystal, atom O1 acts as a bifurcated acceptor, forming inversion-related C10—H10···O1^{i} and C13—H13···O1^{ii} hydrogen bonds that enclose $R_2^2(12)$ and $R_2^2(14)$ rings respectively. These contacts link the molecules into zigzag chains parallel to (10$\bar{1}$) (Table 1

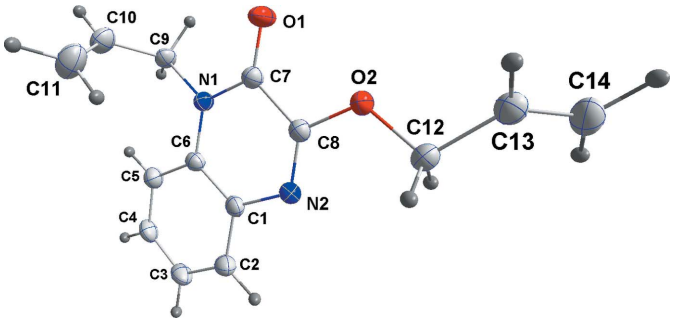


Figure 1
The structure of title molecule, showing the atom-labelling scheme, with ellipsoids drawn at the 50% probability level.

and Fig. 2). Inversion-related C12—H12*B*···*Cg*2^{iii} interactions (Table 1 and Fig. 2) bind two neighboring chains together and these paired chains are further associated through offset π-stacking interactions between head-to-tail pairs of dihydroquinoxaline units [*Cg*1···*Cg*2 = 3.8484 (8) Å, dihedral angle = 1.38 (6)°; *Cg*1 and *Cg*2 are the centroids of the N1/N2/C1/C6–C8 and C1–C6 rings respectively] (Fig. 2).

Synthesis and crystallization

A mixture of quinoxain-2,3-dione (1 g; 6,17 mmol),K_2CO_3 (1,7 g; 12,33 mmol), allylbromide (1,6 ml; 18,60 mmol) and tetra-*n*-butylammonium bromide as a catalyst in *N*,*N*-dimethylformamide (60 ml) was stirred at room temperature for 48 h. Solvent was removed under reduced pressure and the residue chromatographed on a silica-gel column using hexane and ethyl acetate (80/20) as eluent. Recrystallization of the solid product from ethanol afforded the title compound as colourless crystals.

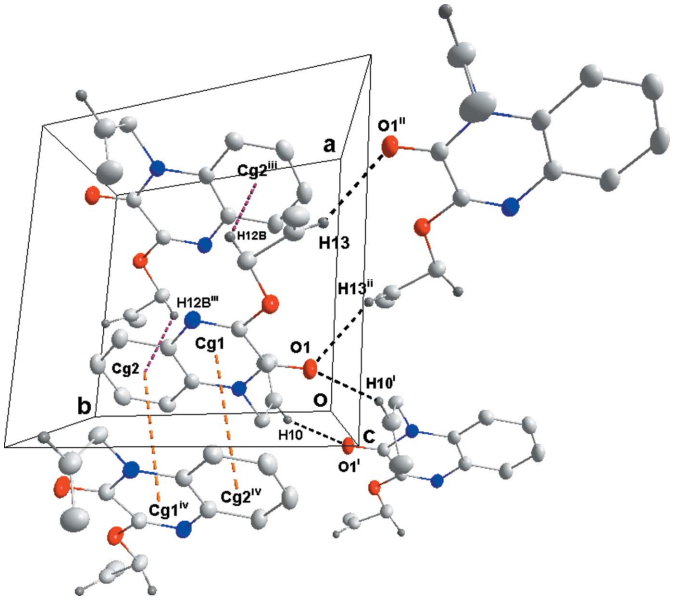


Figure 2
The packing viewed along the *c*-axis direction. C—H···O hydrogen bonds are shown as black dashed lines, while C—H···π(ring) interactions are shown as purple dashed lines. The π-stacking interactions are shown as orange dashed lines. *Cg*1 and *Cg*2 are the centroids of the C1–C6 and C1/C6/N1/C7/C8/N2 rings, respectively. [Symmetry codes (i), (ii) and (iii) are defined in Table 1, while (iv) is $-x, -y+1, -z+1$.]

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

*Cg*2 is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10···O1^{i}	0.97 (2)	2.54 (2)	3.4353 (16)	152.4 (15)
C12—H12*B*···*Cg*2^{ii}	0.984 (17)	2.74 (2)	3.544 (1)	139 (1)
C13—H13···O1^{iii}	0.967 (18)	2.491 (18)	3.2604 (16)	136.4 (14)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_{14}N_2O_2$
M_r	242.27
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	150
a, *b*, *c* (Å)	8.4015 (6), 9.0041 (6), 9.1465 (7)
α, β, γ (°)	114.214 (3), 101.275 (4), 90.978 (3)
V (Å^3)	615.19 (8)
Z	2
Radiation type	Cu *K*α
μ (mm^{-1})	0.72
Crystal size (mm)	0.19 × 0.17 × 0.05
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.84, 0.97
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	4854, 2344, 2090
R_{int}	0.024
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.041, 0.112, 1.06
No. of reflections	2344
No. of parameters	219
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.20, −0.27

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x170656 [https://doi.org/10.1107/S2414314617006563]

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Crystal data

$C_{14}H_{14}N_2O_2$
M_r = 242.27
Triclinic, $P\overline{1}$
a = 8.4015 (6) Å
b = 9.0041 (6) Å
c = 9.1465 (7) Å
α = 114.214 (3)°
β = 101.275 (4)°
γ = 90.978 (3)°
V = 615.19 (8) Å^3
Z = 2
$F(000)$ = 256
D_x = 1.308 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 4058 reflections
θ = 5.4–74.5°
μ = 0.72 mm^{-1}
T = 150 K
Plate, colourless
0.19 × 0.17 × 0.05 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 (*SADABS*; Bruker, 2016)
T_{min} = 0.84, T_{max} = 0.97
4854 measured reflections
2344 independent reflections
2090 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 74.5°, θ_{min} = 5.4°
h = −10→10
k = −11→10
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.112
S = 1.06
2344 reflections
219 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
$w = 1/[\sigma^2(F_o^2) + (0.058P)^2 + 0.1639P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Special details

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	0.17021 (12)	0.09718 (10)	0.33041 (12)	0.0308 (2)
O2	0.38667 (11)	0.24075 (10)	0.61136 (11)	0.0257 (2)
N1	0.11292 (12)	0.34249 (12)	0.32610 (13)	0.0215 (2)
N2	0.35558 (12)	0.49626 (12)	0.61668 (13)	0.0227 (2)
C1	0.27145 (15)	0.58701 (14)	0.54019 (15)	0.0221 (3)
C2	0.31123 (16)	0.75694 (15)	0.61000 (16)	0.0265 (3)
H2	0.397 (2)	0.804 (2)	0.709 (2)	0.036 (4)*
C3	0.22833 (18)	0.85253 (16)	0.54246 (17)	0.0297 (3)
H3	0.260 (2)	0.971 (2)	0.592 (2)	0.033 (4)*
C4	0.10465 (17)	0.77887 (16)	0.40083 (17)	0.0282 (3)
H4	0.047 (2)	0.844 (2)	0.355 (2)	0.045 (5)*
C5	0.06517 (16)	0.61093 (16)	0.32696 (16)	0.0261 (3)
H5	−0.015 (2)	0.561 (2)	0.225 (2)	0.036 (4)*
C6	0.14787 (14)	0.51286 (14)	0.39596 (15)	0.0215 (3)
C7	0.19495 (15)	0.24637 (15)	0.39248 (15)	0.0225 (3)
C8	0.31766 (14)	0.34077 (15)	0.54840 (15)	0.0218 (3)
C9	−0.01289 (15)	0.25660 (15)	0.17450 (15)	0.0238 (3)
H9A	−0.106 (2)	0.3235 (19)	0.1812 (19)	0.028 (4)*
H9B	−0.0541 (19)	0.1501 (19)	0.1772 (19)	0.028 (4)*
C10	0.04657 (16)	0.22011 (17)	0.02069 (16)	0.0303 (3)
H10	−0.037 (2)	0.162 (2)	−0.079 (2)	0.046 (5)*
C11	0.19630 (19)	0.2551 (2)	0.01212 (19)	0.0403 (4)
H11A	0.284 (2)	0.313 (2)	0.111 (2)	0.043 (5)*
H11B	0.227 (3)	0.227 (2)	−0.096 (3)	0.055 (5)*
C12	0.51603 (15)	0.31527 (15)	0.75823 (16)	0.0263 (3)
H12A	0.4707 (19)	0.3934 (19)	0.8475 (19)	0.026 (4)*
H12B	0.601 (2)	0.376 (2)	0.737 (2)	0.032 (4)*
C13	0.58081 (15)	0.17844 (16)	0.79496 (17)	0.0267 (3)
H13	0.613 (2)	0.092 (2)	0.704 (2)	0.036 (4)*
C14	0.59740 (16)	0.17503 (19)	0.93963 (19)	0.0333 (3)
H14A	0.566 (2)	0.265 (2)	1.034 (2)	0.038 (4)*
H14B	0.641 (2)	0.083 (2)	0.958 (2)	0.037 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0343 (5)	0.0177 (4)	0.0329 (5)	0.0004 (4)	−0.0022 (4)	0.0078 (4)
O2	0.0274 (5)	0.0214 (4)	0.0261 (5)	0.0008 (3)	−0.0026 (4)	0.0117 (4)
N1	0.0213 (5)	0.0202 (5)	0.0216 (5)	0.0008 (4)	0.0027 (4)	0.0085 (4)
N2	0.0251 (5)	0.0212 (5)	0.0221 (5)	0.0004 (4)	0.0041 (4)	0.0100 (4)
C1	0.0255 (6)	0.0226 (6)	0.0214 (6)	0.0021 (5)	0.0076 (5)	0.0113 (5)
C2	0.0323 (7)	0.0219 (6)	0.0241 (6)	−0.0002 (5)	0.0063 (5)	0.0085 (5)
C3	0.0398 (7)	0.0202 (6)	0.0316 (7)	0.0028 (5)	0.0119 (6)	0.0117 (5)
C4	0.0340 (7)	0.0266 (7)	0.0321 (7)	0.0082 (5)	0.0112 (5)	0.0185 (5)
C5	0.0264 (6)	0.0271 (7)	0.0272 (7)	0.0046 (5)	0.0061 (5)	0.0139 (5)
C6	0.0224 (6)	0.0208 (6)	0.0230 (6)	0.0021 (4)	0.0079 (5)	0.0097 (5)
C7	0.0232 (6)	0.0208 (6)	0.0231 (6)	0.0022 (4)	0.0042 (5)	0.0093 (5)
C8	0.0228 (6)	0.0207 (6)	0.0228 (6)	0.0026 (4)	0.0045 (5)	0.0103 (5)
C9	0.0205 (6)	0.0243 (6)	0.0240 (6)	−0.0012 (5)	0.0010 (5)	0.0096 (5)
C10	0.0292 (7)	0.0329 (7)	0.0234 (7)	0.0007 (5)	0.0019 (5)	0.0084 (5)
C11	0.0344 (8)	0.0514 (9)	0.0291 (8)	−0.0005 (7)	0.0104 (6)	0.0097 (7)
C12	0.0251 (6)	0.0252 (6)	0.0248 (7)	−0.0007 (5)	−0.0008 (5)	0.0098 (5)
C13	0.0216 (6)	0.0284 (6)	0.0295 (7)	0.0022 (5)	0.0020 (5)	0.0132 (5)
C14	0.0260 (6)	0.0405 (8)	0.0363 (8)	0.0031 (6)	0.0000 (5)	0.0221 (7)

Geometric parameters (Å, º)

O1—C7	1.2202 (15)	C5—H5	0.962 (18)
O2—C8	1.3385 (15)	C7—C8	1.4900 (17)
O2—C12	1.4494 (15)	C9—C10	1.4960 (19)
N1—C7	1.3713 (16)	C9—H9A	0.993 (16)
N1—C6	1.3982 (15)	C9—H9B	1.026 (16)
N1—C9	1.4688 (15)	C10—C11	1.317 (2)
N2—C8	1.2812 (16)	C10—H10	0.97 (2)
N2—C1	1.3971 (16)	C11—H11A	0.986 (19)
C1—C2	1.3993 (17)	C11—H11B	1.00 (2)
C1—C6	1.4080 (17)	C12—C13	1.4892 (17)
C2—C3	1.3769 (19)	C12—H12A	0.983 (16)
C2—H2	0.970 (18)	C12—H12B	0.984 (17)
C3—C4	1.394 (2)	C13—C14	1.316 (2)
C3—H3	0.981 (17)	C13—H13	0.967 (18)
C4—C5	1.3821 (18)	C14—H14A	1.000 (18)
C4—H4	0.943 (19)	C14—H14B	0.972 (18)
C5—C6	1.4026 (17)		
C8—O2—C12	116.73 (9)	N2—C8—C7	126.24 (11)
C7—N1—C6	122.40 (10)	O2—C8—C7	110.83 (10)
C7—N1—C9	116.37 (10)	N1—C9—C10	113.87 (10)
C6—N1—C9	121.22 (10)	N1—C9—H9A	107.6 (9)
C8—N2—C1	117.14 (10)	C10—C9—H9A	111.8 (9)
N2—C1—C2	118.74 (11)	N1—C9—H9B	106.4 (9)

N2—C1—C6	122.05 (11)	C10—C9—H9B	110.4 (9)
C2—C1—C6	119.20 (11)	H9A—C9—H9B	106.4 (13)
C3—C2—C1	121.01 (12)	C11—C10—C9	126.25 (13)
C3—C2—H2	121.9 (10)	C11—C10—H10	120.2 (11)
C1—C2—H2	117.0 (10)	C9—C10—H10	113.5 (11)
C2—C3—C4	119.59 (12)	C10—C11—H11A	122.6 (11)
C2—C3—H3	119.8 (10)	C10—C11—H11B	121.9 (12)
C4—C3—H3	120.5 (10)	H11A—C11—H11B	115.5 (16)
C5—C4—C3	120.71 (12)	O2—C12—C13	106.27 (10)
C5—C4—H4	119.4 (12)	O2—C12—H12A	108.9 (9)
C3—C4—H4	119.9 (12)	C13—C12—H12A	112.5 (9)
C4—C5—C6	120.05 (12)	O2—C12—H12B	109.2 (10)
C4—C5—H5	119.7 (10)	C13—C12—H12B	111.7 (10)
C6—C5—H5	120.2 (10)	H12A—C12—H12B	108.2 (14)
N1—C6—C5	122.36 (11)	C14—C13—C12	123.59 (13)
N1—C6—C1	118.22 (11)	C14—C13—H13	121.8 (10)
C5—C6—C1	119.41 (11)	C12—C13—H13	114.6 (10)
O1—C7—N1	123.43 (11)	C13—C14—H14A	122.2 (10)
O1—C7—C8	122.73 (11)	C13—C14—H14B	120.4 (10)
N1—C7—C8	113.85 (10)	H14A—C14—H14B	117.4 (14)
N2—C8—O2	122.93 (11)		

C8—N2—C1—C2	−179.10 (11)	C6—N1—C7—O1	−177.41 (11)
C8—N2—C1—C6	1.18 (18)	C9—N1—C7—O1	1.48 (18)
N2—C1—C2—C3	−177.86 (11)	C6—N1—C7—C8	2.70 (17)
C6—C1—C2—C3	1.87 (19)	C9—N1—C7—C8	−178.41 (10)
C1—C2—C3—C4	−1.1 (2)	C1—N2—C8—O2	−178.49 (10)
C2—C3—C4—C5	−0.4 (2)	C1—N2—C8—C7	1.61 (19)
C3—C4—C5—C6	1.1 (2)	C12—O2—C8—N2	−3.60 (18)
C7—N1—C6—C5	179.27 (11)	C12—O2—C8—C7	176.30 (10)
C9—N1—C6—C5	0.43 (18)	O1—C7—C8—N2	176.57 (12)
C7—N1—C6—C1	−0.35 (18)	N1—C7—C8—N2	−3.54 (19)
C9—N1—C6—C1	−179.18 (10)	O1—C7—C8—O2	−3.33 (18)
C4—C5—C6—N1	−179.89 (11)	N1—C7—C8—O2	176.56 (10)
C4—C5—C6—C1	−0.28 (19)	C7—N1—C9—C10	−94.54 (13)
N2—C1—C6—N1	−1.83 (18)	C6—N1—C9—C10	84.37 (14)
C2—C1—C6—N1	178.45 (11)	N1—C9—C10—C11	1.2 (2)
N2—C1—C6—C5	178.54 (11)	C8—O2—C12—C13	−175.46 (10)
C2—C1—C6—C5	−1.18 (18)	O2—C12—C13—C14	−128.35 (13)

Hydrogen-bond geometry (Å, º)

Cg2 is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10···O1^{i}	0.97 (2)	2.54 (2)	3.4353 (16)	152.4 (15)

C12—H12*B*···*Cg*2^{ii}	0.984 (17)	2.74 (2)	3.544 (1)	139 (1)
C13—H13···O1^{iii}	0.967 (18)	2.491 (18)	3.2604 (16)	136.4 (14)

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