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1-Benzyl-3-methylquinoxalin-2(1*H*)-one

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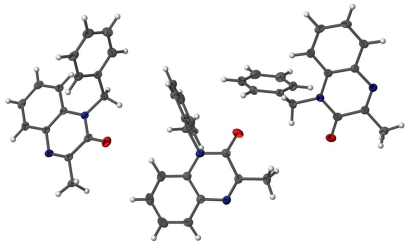
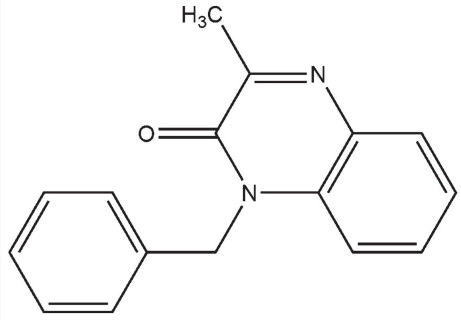
The asymmetric unit of the title compound, $C_{16}H_{14}N_2O$, contains three independent molecules differing primarily in the orientations of the benzyl groups. Each independent molecule forms inversion related dimers *via* offset π-stacking interactions. For two of these dimers, stacks are formed approximately along the *a*-axis direction by a combinations of C—H···N and C—H···π(ring) contacts, in addition to the offset π-stacking interactions. The third set of dimers are also stacked in the same direction but only by pairwise C—H···N hydrogen bonds.

3D view



Chemical scheme



Structure description

Quinoxaline derivatives have a special place in medicinal chemistry and are commonly present in the bioactive molecules used in many therapeutic areas (Kour *et al.*, 2013). Compounds containing the quinoxaline moiety show a wide range of biological activities including anti-inflammatory, analgesic, and antidepressant effects. They also demonstrate antifungal, antibacterial, antimalarial, antitubercular, anticancer, antidiabetic, anti-convulsant, antianxiety, and metal-binding properties (Rohde *et al.*, 2016; Wang *et al.*, 2007; Bérubé *et al.*, 2015; Ramli & Essassi, 2015). In light of the above and as a continuation of our work on the synthesis of quinoxaline-2-thione derivatives in order to evaluate their pharmacological activity (Ramli *et al.*, 2011, 2013, 2017; Caleb *et al.*, 2016), the title compound (Fig. 1) was synthesized and its structure is reported here.

The asymmetric unit of the title compound (Fig. 1) consists of three independent molecules differing primarily in the orientations of the benzyl group. Thus the C1—N2—C10—C11, the C17—N4—C26—C27 and the C33—N6—C42—C43 torsion angles are, respectively, 75.76 (13), 76.68 (13) and −82.29 (13)°.

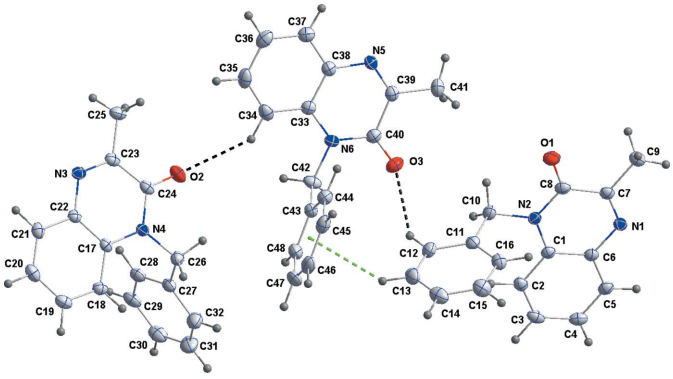


Figure 1
The asymmetric unit with numbering scheme and 50% probability ellipsoids. C—H···O and C—H···π hydrogen bonds are drawn as black and green dashed lines, respectively.

In the crystal, each independent molecule forms a stack, with each stack oriented approximately along the *a*-axis direction (Fig. 2). The O1- and O2-containing molecules form

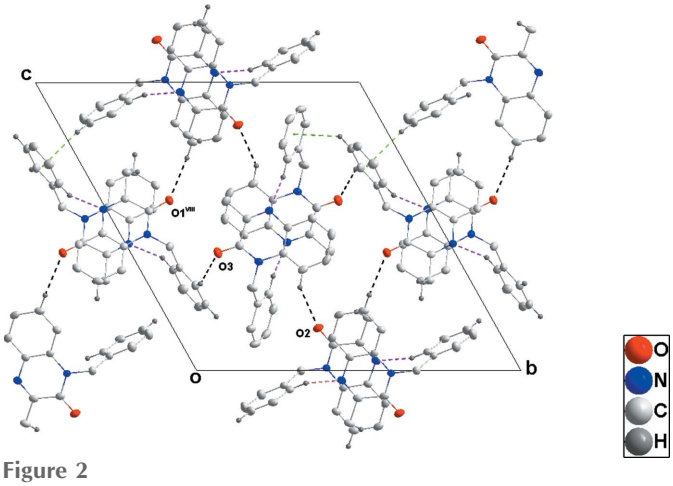


Figure 2
Packing viewed along the *a*-axis direction with hydrogen bonds and C—H···π(ring) interactions depicted as in Fig. 2. [Symmetry code: (viii) $x+1$, y, $z+1$.]

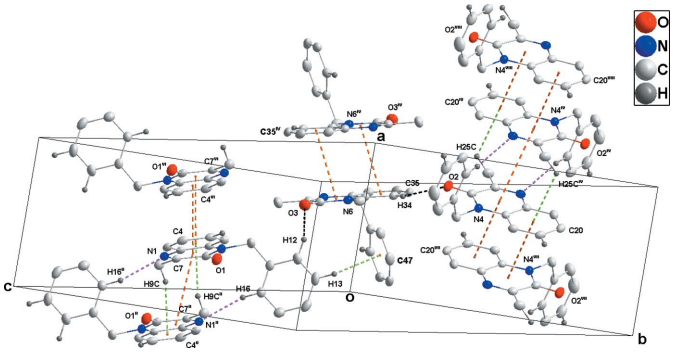


Figure 3
View of the intermolecular interactions. C—H···O and C—H···N hydrogen bonds are shown, respectively, as black and pink dashed lines while π-stacking and C—H···π(ring) interactions are shown, respectively, by orange and green dashed lines. [Symmetry codes: (ii) $-x$, $-y$, $-z+1$; (iv) $-x+2$, $-y+1$, $-z$; (vi) $-x+1$, $-y$, $-z+1$; (vii) $-x+1$, $-y+1$, $-z$; (viii) $x+1$, y, $z+1$.]

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

*Cg*2, *Cg*3, *Cg*6, *Cg*7 and *Cg*11 are the centroids of the C1–C6, C11–C16, C17–C22, C27–C32 and C43–C48 benzene rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···*Cg*7^{i}	1.002 (13)	2.867 (13)	3.6440 (13)	134.8 (11)
C9—H9*C*···*Cg*2^{ii}	0.986 (16)	2.746 (13)	3.4470 (14)	128.4 (13)
C12—H12···O3	0.999 (15)	2.429 (14)	3.2448 (16)	138.5 (10)
C13—H13···*Cg*11	0.961 (16)	2.718 (19)	3.5058 (17)	139.8 (13)
C16—H16···N1^{ii}	0.948 (14)	2.457 (15)	3.3430 (16)	155.5 (11)
C19—H19···O1^{iii}	0.953 (13)	2.553 (14)	3.5016 (14)	174.1 (11)
C25—H25*C*···*Cg*6^{iv}	1.000 (16)	2.835 (15)	3.4591 (14)	121.3 (12)
C28—H28···N3^{iv}	0.990 (13)	2.538 (14)	3.4672 (16)	156.3 (10)
C30—H30···*Cg*3^{i}	1.008 (14)	2.636 (16)	3.5668 (15)	153.9 (12)
C34—H34···O2	0.976 (14)	2.575 (14)	3.4126 (15)	144.0 (11)
C44—H44···N5^{v}	0.988 (13)	2.490 (13)	3.3333 (15)	143.1 (10)

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

head-to-tail inversion dimers through offset π-stacking interactions. For the O1 molecule, the centroid–centroid distance between the C1–C6 and C1/N2/C8/C7/N1/C6 rings is 3.4250 (7) Å. These dimers are further interconnected by inversion-related C16—H16···N1 hydrogen bonds together with pairwise C9—H9*C*···*Cg*2 contacts, Table 1. These impose additional offset π-stacking interactions between the alternating C1/N2/C8/C7/N1/C6 rings [centroid–centroid distance = 3.7405 (7) Å; Fig. 3 (left side)]. A closely similar stacking motif is found for the O2-containing molecules. However the

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{14}N_2O$
M_r	250.29
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, b, c (Å)	7.3502 (4), 17.3508 (10), 17.9449 (10)
α, β, γ (°)	118.226 (1), 100.042 (1), 92.294 (1)
V (Å^3)	1965.63 (19)
Z	6
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.33 × 0.27 × 0.24
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.88, 0.98
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	36858, 9752, 7343
R_{int}	0.032
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.669
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.045, 0.124, 1.04
No. of reflections	9752
No. of parameters	682
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.40, −0.19

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

centroid–centroid distance in the dimer [3.4734 (7) Å] is slightly longer, as are the comparable C25—H25*C*···*Cg*6 and C34—H34···N3 distances [Table 1 and Fig. 2 (right side)]. The additional centroid–centroid distance between the two C17/C22/N3/C23/C24/N4 rings is also longer at 3.8725 (7) Å. Finally, for the O3-containing molecules, dimers are formed with a centroid–centroid distance between the C33–C38 and C33/C38/N5/C39/C40/N6 rings of 3.4811 (7) Å [Fig. 2 (center)]. These dimers are connected only by pairwise C44—H44···N5 hydrogen bonds (Table 1) with no additional C—H···π(ring) or π–π contacts. Stacks of O1- and O2-containing molecules are linked by C19—H19···O1 hydrogen bonds while stacks of the O3-containing molecules are connected to the others by C12—H12···O3 and C34—H34···O2 hydrogen bonds, respectively (Table 1 and Fig. 3).

Synthesis and crystallization

To a solution of 3-methyl-quinoxalin-2(1*H*)-one (0.5 g, 3 mmol) in *N*,*N*-dimethylformamide (20 ml) were added benzyl chloride (0.35 ml, 3 mmol), potassium carbonate (0.43 g, 3 mmol) and a catalytic quantity of tetra-*n*-butyl-ammonium iodide. The mixture was stirred at room temperature for 48 h. The solution was filtered and the solvent removed under reduced pressure. The residue was crystallized from ethanol to afford the title compound as colourless crystals.

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**, x180390 [https://doi.org/10.1107/S2414314618003905]

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Crystal data

$C_{16}H_{14}N_2O$
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Triclinic, $P\overline{1}$
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c = 17.9449 (10) Å
α = 118.226 (1)°
β = 100.042 (1)°
γ = 92.294 (1)°
V = 1965.63 (19) Å^3
Z = 6
$F(000)$ = 792
D_x = 1.269 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9979 reflections
θ = 2.3–28.4°
μ = 0.08 mm^{-1}
T = 100 K
Block, colourless
0.33 × 0.27 × 0.24 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} = 0.88, T_{max} = 0.98
36858 measured reflections
9752 independent reflections
7343 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 28.4°, θ_{min} = 2.3°
h = −9→9
k = −23→23
l = −23→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.124
S = 1.04
9752 reflections
682 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
$w = 1/[\sigma^2(F_o^2) + (0.079P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.25912 (12)	0.20951 (5)	0.59094 (5)	0.0277 (2)
N1	0.21470 (13)	−0.00884 (6)	0.56016 (6)	0.0194 (2)
N2	0.29459 (13)	0.08246 (6)	0.47301 (6)	0.0195 (2)
C1	0.28682 (15)	−0.00957 (7)	0.43184 (7)	0.0179 (2)
C2	0.31828 (16)	−0.05831 (8)	0.34823 (7)	0.0215 (2)
H2	0.3438 (19)	−0.0299 (8)	0.3147 (9)	0.029 (4)*
C3	0.31140 (16)	−0.14907 (8)	0.31127 (7)	0.0237 (2)
H3	0.3302 (18)	−0.1825 (8)	0.2505 (8)	0.026 (3)*
C4	0.27393 (16)	−0.19281 (7)	0.35604 (7)	0.0233 (2)
H4	0.2685 (18)	−0.2559 (9)	0.3295 (8)	0.025 (3)*
C5	0.23991 (16)	−0.14547 (7)	0.43800 (7)	0.0208 (2)
H5	0.2113 (19)	−0.1747 (9)	0.4715 (9)	0.029 (3)*
C6	0.24551 (15)	−0.05360 (7)	0.47658 (7)	0.0184 (2)
C7	0.22057 (15)	0.07611 (7)	0.59656 (7)	0.0189 (2)
C8	0.25818 (15)	0.12892 (7)	0.55450 (7)	0.0202 (2)
C9	0.19308 (18)	0.12631 (8)	0.68734 (8)	0.0245 (3)
H9A	0.306 (3)	0.1689 (10)	0.7257 (11)	0.053 (5)*
H9B	0.168 (2)	0.0877 (10)	0.7109 (10)	0.038 (4)*
H9C	0.089 (2)	0.1611 (10)	0.6900 (10)	0.050 (5)*
C10	0.35018 (17)	0.13201 (8)	0.43105 (8)	0.0236 (2)
H10A	0.4637 (19)	0.1114 (8)	0.4100 (8)	0.026 (3)*
H10B	0.3824 (19)	0.1958 (9)	0.4787 (9)	0.027 (3)*
C11	0.20033 (17)	0.12470 (7)	0.35751 (7)	0.0217 (2)
C12	0.25335 (19)	0.14397 (8)	0.29634 (8)	0.0269 (3)
H12	0.388 (2)	0.1614 (9)	0.3015 (9)	0.031 (4)*
C13	0.1197 (2)	0.14019 (8)	0.22947 (8)	0.0309 (3)
H13	0.157 (2)	0.1535 (10)	0.1877 (10)	0.042 (4)*
C14	−0.0673 (2)	0.11708 (8)	0.22232 (8)	0.0310 (3)
H14	−0.1662 (19)	0.1130 (9)	0.1739 (9)	0.030 (4)*
C15	−0.12054 (19)	0.09877 (8)	0.28310 (8)	0.0299 (3)
H15	−0.256 (2)	0.0797 (9)	0.2770 (10)	0.039 (4)*
C16	0.01263 (17)	0.10252 (8)	0.35061 (8)	0.0250 (3)
H16	−0.0264 (19)	0.0896 (9)	0.3916 (9)	0.031 (4)*
O2	0.83756 (12)	0.44828 (6)	0.14776 (5)	0.0288 (2)
N3	0.82391 (13)	0.56950 (6)	0.03367 (6)	0.0203 (2)
N4	0.68101 (13)	0.40490 (6)	0.00926 (6)	0.0183 (2)

C17	0.64388 (15)	0.42244 (7)	−0.05980 (7)	0.0166 (2)
C18	0.53684 (15)	0.36034 (7)	−0.14181 (7)	0.0203 (2)
H18	0.4877 (19)	0.3022 (9)	−0.1507 (8)	0.029 (4)*
C19	0.50247 (16)	0.38126 (8)	−0.20784 (7)	0.0226 (2)
H19	0.4289 (19)	0.3372 (9)	−0.2623 (9)	0.027 (3)*
C20	0.57138 (16)	0.46423 (8)	−0.19377 (7)	0.0233 (2)
H20	0.5407 (19)	0.4772 (8)	−0.2406 (9)	0.029 (4)*
C21	0.67822 (17)	0.52534 (8)	−0.11371 (7)	0.0219 (2)
H21	0.7310 (19)	0.5837 (9)	−0.1041 (8)	0.026 (3)*
C22	0.71649 (15)	0.50512 (7)	−0.04612 (7)	0.0176 (2)
C23	0.86029 (15)	0.55100 (7)	0.09630 (7)	0.0200 (2)
C24	0.79521 (15)	0.46502 (7)	0.08829 (7)	0.0197 (2)
C25	0.97279 (18)	0.61937 (8)	0.18262 (8)	0.0258 (3)
H25A	0.900 (2)	0.6396 (9)	0.2251 (9)	0.036 (4)*
H25B	1.013 (2)	0.6728 (10)	0.1804 (10)	0.045 (4)*
H25C	1.077 (2)	0.5944 (10)	0.2035 (10)	0.044 (4)*
C26	0.59944 (17)	0.32168 (7)	−0.00011 (8)	0.0223 (2)
H26A	0.605 (2)	0.3317 (9)	0.0589 (10)	0.033 (4)*
H26B	0.4654 (19)	0.3103 (8)	−0.0276 (8)	0.023 (3)*
C27	0.69508 (17)	0.24355 (7)	−0.05122 (7)	0.0215 (2)
C28	0.87161 (17)	0.25453 (8)	−0.06534 (7)	0.0231 (2)
H28	0.9364 (19)	0.3148 (9)	−0.0435 (8)	0.026 (3)*
C29	0.95776 (19)	0.18102 (8)	−0.10981 (7)	0.0273 (3)
H29	1.083 (2)	0.1914 (9)	−0.1200 (9)	0.033 (4)*
C30	0.8698 (2)	0.09670 (8)	−0.13975 (8)	0.0329 (3)
H30	0.932 (2)	0.0436 (9)	−0.1720 (9)	0.038 (4)*
C31	0.6934 (2)	0.08534 (9)	−0.12627 (9)	0.0385 (3)
H31	0.634 (2)	0.0259 (11)	−0.1465 (10)	0.051 (5)*
C32	0.6049 (2)	0.15839 (8)	−0.08264 (9)	0.0327 (3)
H32	0.478 (2)	0.1501 (10)	−0.0735 (10)	0.045 (4)*
O3	0.64780 (13)	0.26946 (5)	0.40946 (6)	0.0306 (2)
N5	0.76117 (13)	0.49974 (6)	0.55516 (6)	0.0207 (2)
N6	0.71477 (13)	0.37944 (6)	0.37836 (6)	0.0201 (2)
C33	0.75948 (15)	0.46950 (7)	0.40722 (7)	0.0191 (2)
C34	0.78126 (16)	0.50245 (8)	0.35079 (8)	0.0242 (2)
H34	0.7675 (19)	0.4622 (9)	0.2889 (9)	0.029 (3)*
C35	0.82796 (17)	0.59192 (9)	0.38409 (9)	0.0279 (3)
H35	0.8423 (19)	0.6146 (9)	0.3469 (9)	0.029 (3)*
C36	0.85515 (17)	0.65104 (8)	0.47278 (9)	0.0281 (3)
H36	0.891 (2)	0.7136 (9)	0.4944 (9)	0.033 (4)*
C37	0.83184 (17)	0.61908 (8)	0.52814 (8)	0.0234 (2)
H37	0.8481 (19)	0.6572 (9)	0.5903 (9)	0.029 (3)*
C38	0.78320 (15)	0.52840 (7)	0.49630 (7)	0.0195 (2)
C39	0.71728 (16)	0.41640 (7)	0.52664 (7)	0.0211 (2)
C40	0.68970 (16)	0.34819 (7)	0.43423 (7)	0.0215 (2)
C41	0.6911 (2)	0.38403 (9)	0.58826 (9)	0.0291 (3)
H41A	0.762 (2)	0.3343 (10)	0.5804 (10)	0.041 (4)*
H41B	0.559 (2)	0.3606 (10)	0.5773 (10)	0.048 (4)*

H41C	0.732 (2)	0.4319 (10)	0.6481 (11)	0.045 (4)*
C42	0.69186 (17)	0.31401 (8)	0.28656 (7)	0.0252 (3)
H42A	0.7162 (18)	0.2580 (9)	0.2844 (8)	0.027 (3)*
H42B	0.788 (2)	0.3291 (8)	0.2620 (9)	0.029 (4)*
C43	0.50068 (16)	0.30338 (7)	0.23189 (7)	0.0211 (2)
C44	0.36495 (17)	0.35469 (8)	0.26581 (8)	0.0236 (2)
H44	0.3899 (18)	0.3989 (9)	0.3280 (9)	0.026 (3)*
C45	0.19109 (18)	0.34284 (8)	0.21381 (9)	0.0279 (3)
H45	0.095 (2)	0.3820 (9)	0.2385 (9)	0.037 (4)*
C46	0.14965 (19)	0.27846 (9)	0.12749 (8)	0.0309 (3)
H46	0.030 (2)	0.2697 (9)	0.0929 (9)	0.036 (4)*
C47	0.2840 (2)	0.22663 (9)	0.09300 (8)	0.0328 (3)
H47	0.257 (2)	0.1820 (10)	0.0335 (11)	0.044 (4)*
C48	0.45847 (18)	0.23918 (8)	0.14456 (8)	0.0269 (3)
H48	0.551 (2)	0.2010 (9)	0.1180 (9)	0.030 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0357 (5)	0.0181 (4)	0.0258 (4)	0.0043 (3)	0.0032 (4)	0.0090 (3)
N1	0.0185 (5)	0.0203 (4)	0.0177 (4)	0.0015 (4)	0.0023 (4)	0.0086 (4)
N2	0.0207 (5)	0.0179 (4)	0.0193 (5)	0.0004 (4)	0.0020 (4)	0.0095 (4)
C1	0.0136 (5)	0.0195 (5)	0.0188 (5)	0.0011 (4)	0.0005 (4)	0.0089 (4)
C2	0.0182 (6)	0.0264 (6)	0.0198 (5)	0.0021 (4)	0.0026 (4)	0.0118 (5)
C3	0.0178 (6)	0.0274 (6)	0.0178 (5)	0.0050 (5)	0.0017 (4)	0.0052 (5)
C4	0.0205 (6)	0.0183 (5)	0.0232 (6)	0.0036 (4)	−0.0008 (5)	0.0056 (5)
C5	0.0173 (6)	0.0200 (5)	0.0228 (6)	0.0005 (4)	−0.0010 (4)	0.0105 (5)
C6	0.0143 (5)	0.0204 (5)	0.0181 (5)	0.0015 (4)	0.0002 (4)	0.0086 (4)
C7	0.0137 (5)	0.0223 (5)	0.0180 (5)	0.0013 (4)	−0.0003 (4)	0.0092 (4)
C8	0.0181 (6)	0.0195 (5)	0.0196 (5)	0.0022 (4)	−0.0009 (4)	0.0085 (4)
C9	0.0254 (7)	0.0255 (6)	0.0194 (6)	0.0038 (5)	0.0036 (5)	0.0088 (5)
C10	0.0243 (6)	0.0242 (6)	0.0245 (6)	−0.0013 (5)	0.0032 (5)	0.0147 (5)
C11	0.0277 (6)	0.0157 (5)	0.0209 (5)	0.0034 (4)	0.0051 (5)	0.0084 (4)
C12	0.0335 (7)	0.0221 (6)	0.0275 (6)	0.0002 (5)	0.0078 (5)	0.0138 (5)
C13	0.0472 (9)	0.0239 (6)	0.0268 (6)	0.0059 (5)	0.0083 (6)	0.0163 (5)
C14	0.0415 (8)	0.0260 (6)	0.0249 (6)	0.0135 (5)	0.0029 (6)	0.0128 (5)
C15	0.0276 (7)	0.0318 (6)	0.0299 (7)	0.0099 (5)	0.0062 (5)	0.0145 (5)
C16	0.0276 (7)	0.0263 (6)	0.0247 (6)	0.0063 (5)	0.0079 (5)	0.0144 (5)
O2	0.0324 (5)	0.0361 (5)	0.0211 (4)	0.0093 (4)	0.0047 (4)	0.0165 (4)
N3	0.0183 (5)	0.0192 (4)	0.0191 (5)	0.0026 (4)	0.0053 (4)	0.0056 (4)
N4	0.0203 (5)	0.0179 (4)	0.0161 (4)	0.0033 (4)	0.0042 (4)	0.0077 (4)
C17	0.0152 (5)	0.0195 (5)	0.0158 (5)	0.0057 (4)	0.0057 (4)	0.0081 (4)
C18	0.0180 (6)	0.0204 (5)	0.0190 (5)	0.0032 (4)	0.0044 (4)	0.0065 (4)
C19	0.0177 (6)	0.0282 (6)	0.0168 (5)	0.0067 (5)	0.0031 (4)	0.0070 (5)
C20	0.0228 (6)	0.0328 (6)	0.0197 (5)	0.0122 (5)	0.0082 (5)	0.0153 (5)
C21	0.0236 (6)	0.0233 (5)	0.0237 (6)	0.0079 (5)	0.0102 (5)	0.0134 (5)
C22	0.0157 (5)	0.0185 (5)	0.0167 (5)	0.0040 (4)	0.0057 (4)	0.0062 (4)
C23	0.0167 (5)	0.0225 (5)	0.0174 (5)	0.0050 (4)	0.0058 (4)	0.0062 (4)

C24	0.0171 (5)	0.0245 (5)	0.0164 (5)	0.0070 (4)	0.0051 (4)	0.0084 (4)
C25	0.0223 (6)	0.0268 (6)	0.0185 (6)	0.0013 (5)	0.0028 (5)	0.0041 (5)
C26	0.0264 (7)	0.0195 (5)	0.0226 (6)	0.0040 (5)	0.0094 (5)	0.0103 (5)
C27	0.0299 (6)	0.0192 (5)	0.0164 (5)	0.0055 (4)	0.0054 (5)	0.0093 (4)
C28	0.0272 (6)	0.0240 (6)	0.0166 (5)	0.0055 (5)	0.0015 (5)	0.0096 (5)
C29	0.0299 (7)	0.0319 (6)	0.0176 (5)	0.0109 (5)	0.0031 (5)	0.0104 (5)
C30	0.0489 (9)	0.0250 (6)	0.0248 (6)	0.0157 (6)	0.0091 (6)	0.0111 (5)
C31	0.0591 (10)	0.0203 (6)	0.0363 (8)	0.0065 (6)	0.0166 (7)	0.0121 (6)
C32	0.0421 (8)	0.0249 (6)	0.0330 (7)	0.0035 (6)	0.0138 (6)	0.0139 (5)
O3	0.0319 (5)	0.0207 (4)	0.0352 (5)	−0.0005 (4)	0.0054 (4)	0.0114 (4)
N5	0.0208 (5)	0.0230 (5)	0.0196 (5)	0.0052 (4)	0.0055 (4)	0.0108 (4)
N6	0.0197 (5)	0.0198 (4)	0.0176 (5)	0.0036 (4)	0.0036 (4)	0.0067 (4)
C33	0.0153 (5)	0.0213 (5)	0.0206 (5)	0.0043 (4)	0.0026 (4)	0.0105 (4)
C34	0.0185 (6)	0.0355 (6)	0.0218 (6)	0.0048 (5)	0.0022 (5)	0.0171 (5)
C35	0.0216 (6)	0.0387 (7)	0.0359 (7)	0.0055 (5)	0.0035 (5)	0.0289 (6)
C36	0.0236 (6)	0.0241 (6)	0.0399 (7)	0.0044 (5)	0.0025 (5)	0.0197 (6)
C37	0.0217 (6)	0.0217 (5)	0.0250 (6)	0.0053 (4)	0.0034 (5)	0.0103 (5)
C38	0.0165 (5)	0.0221 (5)	0.0210 (5)	0.0051 (4)	0.0043 (4)	0.0112 (5)
C39	0.0179 (6)	0.0247 (5)	0.0228 (6)	0.0045 (4)	0.0057 (4)	0.0128 (5)
C40	0.0183 (6)	0.0219 (5)	0.0240 (6)	0.0031 (4)	0.0034 (4)	0.0112 (5)
C41	0.0318 (7)	0.0330 (7)	0.0300 (7)	0.0032 (6)	0.0115 (6)	0.0198 (6)
C42	0.0236 (6)	0.0261 (6)	0.0191 (6)	0.0071 (5)	0.0054 (5)	0.0051 (5)
C43	0.0235 (6)	0.0213 (5)	0.0189 (5)	0.0009 (4)	0.0040 (4)	0.0105 (4)
C44	0.0241 (6)	0.0228 (5)	0.0232 (6)	0.0014 (5)	0.0048 (5)	0.0108 (5)
C45	0.0236 (6)	0.0321 (6)	0.0366 (7)	0.0031 (5)	0.0058 (5)	0.0240 (6)
C46	0.0265 (7)	0.0415 (7)	0.0311 (7)	−0.0056 (6)	−0.0038 (6)	0.0269 (6)
C47	0.0394 (8)	0.0381 (7)	0.0183 (6)	−0.0062 (6)	0.0004 (5)	0.0146 (6)
C48	0.0332 (7)	0.0276 (6)	0.0206 (6)	0.0016 (5)	0.0083 (5)	0.0116 (5)

Geometric parameters (Å, º)

O1—C8	1.2311 (13)	C25—H25A	0.948 (15)
N1—C7	1.2944 (14)	C25—H25B	0.981 (16)
N1—C6	1.3909 (14)	C25—H25C	1.000 (16)
N2—C8	1.3779 (14)	C26—C27	1.5159 (15)
N2—C1	1.4004 (13)	C26—H26A	0.983 (15)
N2—C10	1.4711 (15)	C26—H26B	0.988 (14)
C1—C2	1.3986 (15)	C27—C28	1.3874 (17)
C1—C6	1.4026 (15)	C27—C32	1.3939 (17)
C2—C3	1.3843 (16)	C28—C29	1.3938 (16)
C2—H2	0.976 (14)	C28—H28	0.990 (13)
C3—C4	1.3908 (18)	C29—C30	1.3810 (19)
C3—H3	1.002 (13)	C29—H29	0.996 (15)
C4—C5	1.3793 (16)	C30—C31	1.383 (2)
C4—H4	0.961 (13)	C30—H30	1.008 (14)
C5—C6	1.4011 (15)	C31—C32	1.3954 (18)
C5—H5	0.993 (14)	C31—H31	0.970 (16)
C7—C8	1.4805 (16)	C32—H32	0.994 (16)

C7—C9	1.4967 (15)	O3—C40	1.2259 (13)
C9—H9A	0.990 (18)	N5—C39	1.2892 (14)
C9—H9B	0.975 (16)	N5—C38	1.3926 (14)
C9—H9C	0.986 (16)	N6—C40	1.3798 (15)
C10—C11	1.5148 (17)	N6—C33	1.3971 (14)
C10—H10A	0.986 (13)	N6—C42	1.4662 (14)
C10—H10B	1.012 (13)	C33—C38	1.4048 (15)
C11—C16	1.3855 (17)	C33—C34	1.4053 (16)
C11—C12	1.3982 (17)	C34—C35	1.3759 (17)
C12—C13	1.3850 (18)	C34—H34	0.976 (14)
C12—H12	0.999 (15)	C35—C36	1.3977 (18)
C13—C14	1.383 (2)	C35—H35	0.940 (14)
C13—H13	0.961 (16)	C36—C37	1.3772 (18)
C14—C15	1.3821 (19)	C36—H36	0.971 (14)
C14—H14	1.002 (14)	C37—C38	1.4012 (15)
C15—C16	1.3917 (18)	C37—H37	0.972 (14)
C15—H15	1.007 (16)	C39—C40	1.4828 (16)
C16—H16	0.948 (14)	C39—C41	1.4927 (16)
O2—C24	1.2267 (13)	C41—H41A	0.990 (15)
N3—C23	1.2965 (15)	C41—H41B	0.985 (18)
N3—C22	1.3942 (14)	C41—H41C	0.979 (16)
N4—C24	1.3854 (14)	C42—C43	1.5161 (17)
N4—C17	1.3958 (14)	C42—H42A	0.979 (13)
N4—C26	1.4624 (14)	C42—H42B	0.982 (15)
C17—C22	1.4010 (15)	C43—C44	1.3888 (16)
C17—C18	1.4051 (15)	C43—C48	1.3945 (16)
C18—C19	1.3817 (16)	C44—C45	1.3884 (17)
C18—H18	0.986 (14)	C44—H44	0.988 (13)
C19—C20	1.3949 (17)	C45—C46	1.3825 (18)
C19—H19	0.953 (13)	C45—H45	1.009 (14)
C20—C21	1.3798 (17)	C46—C47	1.387 (2)
C20—H20	0.962 (14)	C46—H46	0.946 (15)
C21—C22	1.4018 (15)	C47—C48	1.3862 (19)
C21—H21	0.992 (13)	C47—H47	0.954 (16)
C23—C24	1.4801 (16)	C48—H48	0.991 (14)
C23—C25	1.4924 (16)		

C7—N1—C6	118.37 (10)	C23—C25—H25B	110.3 (9)
C8—N2—C1	121.26 (9)	H25A—C25—H25B	103.6 (12)
C8—N2—C10	118.54 (9)	C23—C25—H25C	110.7 (9)
C1—N2—C10	120.15 (9)	H25A—C25—H25C	106.7 (13)
C2—C1—N2	122.24 (10)	H25B—C25—H25C	114.0 (13)
C2—C1—C6	119.46 (10)	N4—C26—C27	113.64 (10)
N2—C1—C6	118.30 (9)	N4—C26—H26A	106.3 (8)
C3—C2—C1	119.68 (11)	C27—C26—H26A	111.8 (8)
C3—C2—H2	118.8 (8)	N4—C26—H26B	108.7 (7)
C1—C2—H2	121.5 (8)	C27—C26—H26B	110.3 (7)
C2—C3—C4	121.05 (11)	H26A—C26—H26B	105.7 (11)

C2—C3—H3	117.9 (7)	C28—C27—C32	119.23 (11)
C4—C3—H3	121.1 (7)	C28—C27—C26	121.85 (10)
C5—C4—C3	119.69 (10)	C32—C27—C26	118.89 (11)
C5—C4—H4	120.1 (8)	C27—C28—C29	120.10 (12)
C3—C4—H4	120.2 (8)	C27—C28—H28	119.8 (8)
C4—C5—C6	120.25 (11)	C29—C28—H28	120.1 (8)
C4—C5—H5	121.8 (8)	C30—C29—C28	120.69 (13)
C6—C5—H5	118.0 (8)	C30—C29—H29	121.5 (8)
N1—C6—C5	117.89 (10)	C28—C29—H29	117.8 (8)
N1—C6—C1	122.23 (9)	C29—C30—C31	119.45 (11)
C5—C6—C1	119.85 (10)	C29—C30—H30	120.6 (8)
N1—C7—C8	123.90 (10)	C31—C30—H30	119.9 (8)
N1—C7—C9	119.56 (10)	C30—C31—C32	120.36 (13)
C8—C7—C9	116.53 (10)	C30—C31—H31	118.9 (10)
O1—C8—N2	122.39 (10)	C32—C31—H31	120.8 (10)
O1—C8—C7	121.74 (10)	C27—C32—C31	120.15 (13)
N2—C8—C7	115.87 (9)	C27—C32—H32	119.6 (9)
C7—C9—H9A	110.1 (10)	C31—C32—H32	120.2 (9)
C7—C9—H9B	112.4 (9)	C39—N5—C38	118.69 (9)
H9A—C9—H9B	108.1 (13)	C40—N6—C33	121.90 (9)
C7—C9—H9C	110.8 (9)	C40—N6—C42	117.19 (9)
H9A—C9—H9C	106.8 (13)	C33—N6—C42	120.90 (10)
H9B—C9—H9C	108.4 (13)	N6—C33—C38	117.91 (10)
N2—C10—C11	114.25 (10)	N6—C33—C34	122.53 (10)
N2—C10—H10A	108.4 (8)	C38—C33—C34	119.56 (10)
C11—C10—H10A	110.1 (8)	C35—C34—C33	119.27 (11)
N2—C10—H10B	105.3 (8)	C35—C34—H34	120.3 (8)
C11—C10—H10B	109.8 (8)	C33—C34—H34	120.4 (8)
H10A—C10—H10B	108.7 (11)	C34—C35—C36	121.73 (11)
C16—C11—C12	119.09 (11)	C34—C35—H35	119.9 (8)
C16—C11—C10	122.22 (11)	C36—C35—H35	118.4 (8)
C12—C11—C10	118.65 (11)	C37—C36—C35	119.15 (11)
C13—C12—C11	120.27 (13)	C37—C36—H36	121.2 (8)
C13—C12—H12	120.0 (8)	C35—C36—H36	119.7 (8)
C11—C12—H12	119.7 (8)	C36—C37—C38	120.58 (11)
C14—C13—C12	120.42 (12)	C36—C37—H37	122.6 (8)
C14—C13—H13	119.9 (9)	C38—C37—H37	116.8 (8)
C12—C13—H13	119.7 (10)	N5—C38—C37	118.16 (10)
C15—C14—C13	119.52 (12)	N5—C38—C33	122.14 (10)
C15—C14—H14	118.7 (8)	C37—C38—C33	119.70 (10)
C13—C14—H14	121.8 (8)	N5—C39—C40	123.91 (10)
C14—C15—C16	120.50 (13)	N5—C39—C41	119.75 (10)
C14—C15—H15	119.9 (9)	C40—C39—C41	116.33 (10)
C16—C15—H15	119.5 (9)	O3—C40—N6	122.49 (10)
C11—C16—C15	120.20 (12)	O3—C40—C39	122.08 (11)
C11—C16—H16	120.5 (9)	N6—C40—C39	115.43 (9)
C15—C16—H16	119.3 (9)	C39—C41—H41A	111.6 (9)
C23—N3—C22	118.48 (10)	C39—C41—H41B	110.4 (9)

C24—N4—C17	121.54 (9)	H41A—C41—H41B	105.6 (13)
C24—N4—C26	117.97 (9)	C39—C41—H41C	110.2 (9)
C17—N4—C26	120.49 (9)	H41A—C41—H41C	108.9 (12)
N4—C17—C22	118.35 (9)	H41B—C41—H41C	110.0 (13)
N4—C17—C18	122.32 (10)	N6—C42—C43	113.72 (9)
C22—C17—C18	119.33 (10)	N6—C42—H42A	106.6 (8)
C19—C18—C17	120.09 (11)	C43—C42—H42A	110.5 (8)
C19—C18—H18	121.4 (8)	N6—C42—H42B	110.3 (8)
C17—C18—H18	118.5 (8)	C43—C42—H42B	109.3 (8)
C18—C19—C20	120.62 (11)	H42A—C42—H42B	106.1 (11)
C18—C19—H19	117.1 (8)	C44—C43—C48	118.65 (11)
C20—C19—H19	122.2 (8)	C44—C43—C42	122.39 (10)
C21—C20—C19	119.71 (11)	C48—C43—C42	118.95 (10)
C21—C20—H20	122.0 (8)	C45—C44—C43	120.77 (11)
C19—C20—H20	118.3 (8)	C45—C44—H44	119.1 (8)
C20—C21—C22	120.58 (11)	C43—C44—H44	120.1 (8)
C20—C21—H21	119.9 (8)	C46—C45—C44	120.23 (12)
C22—C21—H21	119.5 (8)	C46—C45—H45	119.7 (8)
N3—C22—C17	122.10 (10)	C44—C45—H45	120.1 (8)
N3—C22—C21	118.25 (10)	C45—C46—C47	119.48 (12)
C17—C22—C21	119.64 (10)	C45—C46—H46	119.7 (9)
N3—C23—C24	123.92 (10)	C47—C46—H46	120.8 (9)
N3—C23—C25	119.38 (11)	C48—C47—C46	120.36 (12)
C24—C23—C25	116.70 (10)	C48—C47—H47	119.4 (10)
O2—C24—N4	122.12 (10)	C46—C47—H47	120.3 (10)
O2—C24—C23	122.44 (10)	C47—C48—C43	120.50 (12)
N4—C24—C23	115.43 (9)	C47—C48—H48	118.3 (8)
C23—C25—H25A	111.4 (9)	C43—C48—H48	121.2 (8)

C8—N2—C1—C2	178.23 (10)	C26—N4—C24—O2	4.31 (15)
C10—N2—C1—C2	−4.42 (16)	C17—N4—C24—C23	5.08 (14)
C8—N2—C1—C6	−1.61 (15)	C26—N4—C24—C23	−174.92 (9)
C10—N2—C1—C6	175.74 (10)	N3—C23—C24—O2	177.27 (10)
N2—C1—C2—C3	179.07 (10)	C25—C23—C24—O2	−3.28 (15)
C6—C1—C2—C3	−1.09 (16)	N3—C23—C24—N4	−3.50 (15)
C1—C2—C3—C4	−0.11 (17)	C25—C23—C24—N4	175.95 (9)
C2—C3—C4—C5	1.10 (17)	C24—N4—C26—C27	−103.32 (11)
C3—C4—C5—C6	−0.87 (17)	C17—N4—C26—C27	76.68 (13)
C7—N1—C6—C5	179.64 (10)	N4—C26—C27—C28	17.37 (15)
C7—N1—C6—C1	1.57 (15)	N4—C26—C27—C32	−164.53 (11)
C4—C5—C6—N1	−178.44 (10)	C32—C27—C28—C29	−0.57 (17)
C4—C5—C6—C1	−0.32 (16)	C26—C27—C28—C29	177.52 (10)
C2—C1—C6—N1	179.34 (10)	C27—C28—C29—C30	−0.45 (17)
N2—C1—C6—N1	−0.82 (15)	C28—C29—C30—C31	0.80 (19)
C2—C1—C6—C5	1.31 (16)	C29—C30—C31—C32	−0.1 (2)
N2—C1—C6—C5	−178.85 (9)	C28—C27—C32—C31	1.25 (19)
C6—N1—C7—C8	0.03 (16)	C26—C27—C32—C31	−176.91 (12)
C6—N1—C7—C9	−178.35 (10)	C30—C31—C32—C27	−0.9 (2)

C1—N2—C8—O1	−177.94 (10)	C40—N6—C33—C38	1.53 (16)
C10—N2—C8—O1	4.66 (16)	C42—N6—C33—C38	−178.70 (10)
C1—N2—C8—C7	3.00 (15)	C40—N6—C33—C34	−178.52 (10)
C10—N2—C8—C7	−174.40 (9)	C42—N6—C33—C34	1.26 (16)
N1—C7—C8—O1	178.65 (10)	N6—C33—C34—C35	−179.09 (10)
C9—C7—C8—O1	−2.92 (16)	C38—C33—C34—C35	0.86 (17)
N1—C7—C8—N2	−2.28 (16)	C33—C34—C35—C36	0.26 (18)
C9—C7—C8—N2	176.14 (10)	C34—C35—C36—C37	−1.00 (18)
C8—N2—C10—C11	−106.81 (11)	C35—C36—C37—C38	0.59 (18)
C1—N2—C10—C11	75.76 (13)	C39—N5—C38—C37	−179.68 (10)
N2—C10—C11—C16	22.47 (15)	C39—N5—C38—C33	−0.12 (16)
N2—C10—C11—C12	−159.76 (10)	C36—C37—C38—N5	−179.91 (10)
C16—C11—C12—C13	−0.50 (17)	C36—C37—C38—C33	0.52 (17)
C10—C11—C12—C13	−178.35 (11)	N6—C33—C38—N5	−0.85 (16)
C11—C12—C13—C14	−0.20 (18)	C34—C33—C38—N5	179.20 (10)
C12—C13—C14—C15	0.80 (18)	N6—C33—C38—C37	178.71 (10)
C13—C14—C15—C16	−0.69 (18)	C34—C33—C38—C37	−1.25 (16)
C12—C11—C16—C15	0.61 (17)	C38—N5—C39—C40	0.46 (16)
C10—C11—C16—C15	178.37 (11)	C38—N5—C39—C41	−179.43 (10)
C14—C15—C16—C11	−0.01 (18)	C33—N6—C40—O3	178.91 (10)
C24—N4—C17—C22	−3.62 (15)	C42—N6—C40—O3	−0.87 (16)
C26—N4—C17—C22	176.38 (9)	C33—N6—C40—C39	−1.20 (15)
C24—N4—C17—C18	176.43 (9)	C42—N6—C40—C39	179.02 (10)
C26—N4—C17—C18	−3.57 (15)	N5—C39—C40—O3	−179.93 (11)
N4—C17—C18—C19	179.35 (9)	C41—C39—C40—O3	−0.04 (16)
C22—C17—C18—C19	−0.61 (15)	N5—C39—C40—N6	0.18 (16)
C17—C18—C19—C20	−0.74 (16)	C41—C39—C40—N6	−179.92 (10)
C18—C19—C20—C21	1.39 (16)	C40—N6—C42—C43	97.49 (12)
C19—C20—C21—C22	−0.67 (16)	C33—N6—C42—C43	−82.29 (13)
C23—N3—C22—C17	1.47 (15)	N6—C42—C43—C44	3.16 (17)
C23—N3—C22—C21	−179.74 (9)	N6—C42—C43—C48	−176.14 (11)
N4—C17—C22—N3	0.13 (15)	C48—C43—C44—C45	−0.44 (17)
C18—C17—C22—N3	−179.91 (9)	C42—C43—C44—C45	−179.74 (11)
N4—C17—C22—C21	−178.65 (9)	C43—C44—C45—C46	1.09 (18)
C18—C17—C22—C21	1.31 (15)	C44—C45—C46—C47	−0.87 (18)
C20—C21—C22—N3	−179.50 (10)	C45—C46—C47—C48	0.01 (19)
C20—C21—C22—C17	−0.68 (16)	C46—C47—C48—C43	0.64 (19)
C22—N3—C23—C24	0.29 (15)	C44—C43—C48—C47	−0.42 (18)
C22—N3—C23—C25	−179.15 (10)	C42—C43—C48—C47	178.91 (12)
C17—N4—C24—O2	−175.69 (9)		

Hydrogen-bond geometry (Å, º)

Cg2, Cg3, Cg6, Cg7 and Cg11 are the centroids of the C1–C6, C11–C16, C17–C22, C27–C32 and C43–C48 benzene rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···*Cg*7^{i}	1.002 (13)	2.867 (13)	3.6440 (13)	134.8 (11)
C9—H9*C*···*Cg*2^{ii}	0.986 (16)	2.746 (13)	3.4470 (14)	128.4 (13)
C12—H12···O3	0.999 (15)	2.429 (14)	3.2448 (16)	138.5 (10)

C13—H13···*Cg*11	0.961 (16)	2.718 (19)	3.5058 (17)	139.8 (13)
C16—H16···N1^{ii}	0.948 (14)	2.457 (15)	3.3430 (16)	155.5 (11)
C19—H19···O1^{iii}	0.953 (13)	2.553 (14)	3.5016 (14)	174.1 (11)
C25—H25*C*···*Cg*6^{iv}	1.000 (16)	2.835 (15)	3.4591 (14)	121.3 (12)
C28—H28···N3^{iv}	0.990 (13)	2.538 (14)	3.4672 (16)	156.3 (10)
C30—H30···*Cg*3^{i}	1.008 (14)	2.636 (16)	3.5668 (15)	153.9 (12)
C34—H34···O2	0.976 (14)	2.575 (14)	3.4126 (15)	144.0 (11)
C44—H44···N5^{v}	0.988 (13)	2.490 (13)	3.3333 (15)	143.1 (10)

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