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Crystal structure and Hirshfeld surface analysis of 3-isoamyl-6-nitroquinazolin-4-one

Fazliddin Zulpanov,[a] Muzaffar Davlatboev,[b]* Rajab Samiev,[c] Bakhromjon Juraev,[d] Ubaydullo Yakubov[a] and Burkhon Elmuradov[a]

[a]Institute of the Chemistry of Plant Substances, Uzbekistan Academy of Sciences, Mirzo Ulugbek Str. 77, Tashkent 100170, Uzbekistan, [b]University of Business and Science, Beshkapa street, Namangan 160100, Uzbekistan, [c]Samarkand State University, University blv. 15, Samarkand 140104, Uzbekistan, and [d]Institute of the Chemistry of Plant Substances, Mirzo Ulugbek Str. 77, Tashkent 100170, Uzbekistan. *Correspondence e-mail: davlatboyev.muzaffar@mail.ru

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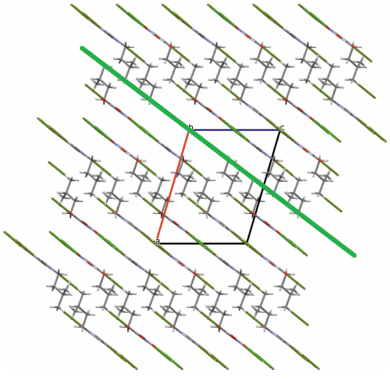
Keywords: 3-isoamyl-6-nitroquinazolin-4-one; crystal structure; hydrogen-bonding; intermolecular interactions; Hirshfeld surface analysis.

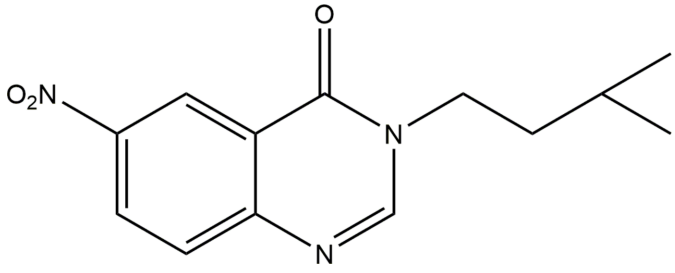
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The title compound [systematic name: 3-(3-methylbutyl)-6-nitro-3,4-dihydroquinazolin-4-one], $C_{13}H_{15}N_3O_3$, crystallizes in the monoclinic space group $P2_1/c$ (Z = 4). In the crystal, molecules are connected through C—H···O and C—H···N hydrogen bonds, forming supramolecular layers parallel to $(\bar{2}01)$. Centroid-to-centroid separations indicate that π–π stacking interactions are negligible. A Hirshfeld surface analysis was performed to quantify the close intermolecular contacts, indicating that H···H (39.2%), O···H/H···O (28.4%), and C···H/H···C (16.0%) interactions represent the main contributors to the crystal packing.

1. Chemical context

Quinazoline and quinazolinone derivatives constitute an important class of nitrogen-containing heterocyclic compounds. Their chemistry and reported biological activities have motivated considerable research (Wu *et al.*, 2011; Singh *et al.*, 2013). Several quinazoline-based compounds, including the epidermal growth factor receptor inhibitors *erlotinib* and *gefitinib*, have been studied in anticancer drug development (Cohen *et al.*, 2005; Petrov *et al.*, 2006; Wu *et al.*, 2010). Structural characterization of related quinazolinone derivatives is valuable for understanding their molecular conformations and solid-state intermolecular interactions. In this context, we report the molecular and crystal structures of 3-isoamyl-6-nitroquinazolin-4-one, (I), accompanied by the results of a Hirshfeld surface analysis.





2. Structural commentary

The molecular structure of (I) comprises a nearly planar bicyclic quinazolinone system (Fig. 1). The root-mean-square (r.m.s.) deviation for the ten non-hydrogen ring atoms (N1, N3, C2, C4, C4*A*, C5, C6, C7, C8, C8*A*) from their mean plane is 0.010 Å, with a maximum deviation of 0.015 (2) Å observed for atom N3. The isoamyl chain attached at atom N3 adopts an

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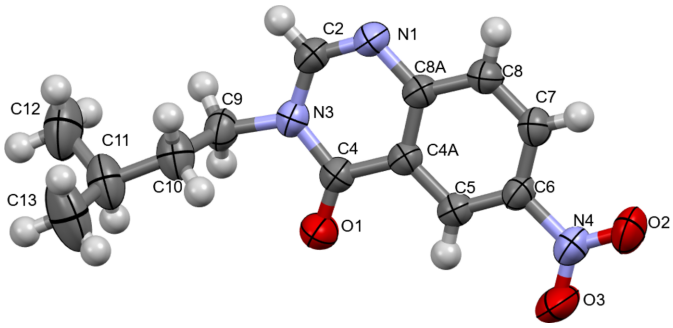


Figure 1
Molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

extended conformation, characterized by the torsion angles N3—C9—C10—C11 = 168.0 (2)°, C9—C10—C11—C12 = 60.6 (3)° and C9—C10—C11—C13 = −172.9 (4)°. The nitro group at position C6 is essentially coplanar with the quinazolinone ring, as shown by the dihedral angle of 1.7 (3)° between the two moieties [torsion angle O2—N4—C6—C7 = 1.3 (2)°].

3. Supramolecular features

In the crystal structure of (I), molecules are linked by intermolecular C—H···O and C—H···N hydrogen bonds (Table 1), forming supramolecular layers parallel to ($\bar{2}$01), Fig. 2. A selection of these non-classical hydrogen-bonding interactions is shown in Fig. 3. Although centroid-to-centroid contacts exist between quinazolinone rings of neighbouring molecules [*e.g.*, *Cg*1···*Cg*2^{i} = 4.7241 (13) Å, symmetry code: (i) $2-x, -\frac{1}{2}+y, \frac{3}{2}-z$; *Cg*1 is the centroid of the N1/C2/N3/C4/C4*A*/C8*A* ring, *Cg*2 is the centroid of the C4*A*/C5–C8/C8*A* ring], the large slippage (3.446 Å) indicates that π–π stacking interactions are negligible and do not contribute significantly to the consolidation of the crystal packing.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H1*c*···O1^{i}	0.96 (3)	2.54 (2)	3.493 (5)	172 (3)
C8—H8···N1^{ii}	0.93 (1)	2.54 (1)	3.462 (3)	169 (1)

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

4. Hirshfeld surface analysis

A Hirshfeld surface (HS) analysis (Hirshfeld, 1977) was carried out using *CrystalExplorer* (Spackman *et al.*, 2021) to visualize and quantify non-covalent interactions in the crystal packing of (I). The HS mapped over d_{norm} is represented in Fig. 4, where the white surface indicates contacts with distances equal to the sum of van der Waals radii, while the red and blue colours indicate distances shorter and longer than the sum of van der Waals radii, respectively. The bright-red spots on the d_{norm} surface originate from intermolecular hydrogen-bonding interactions, with N and O atoms as acceptors and C—H as donor groups.

Two-dimensional fingerprint plots (Spackman & McKinnon, 2002) for the full surface and those delineated into

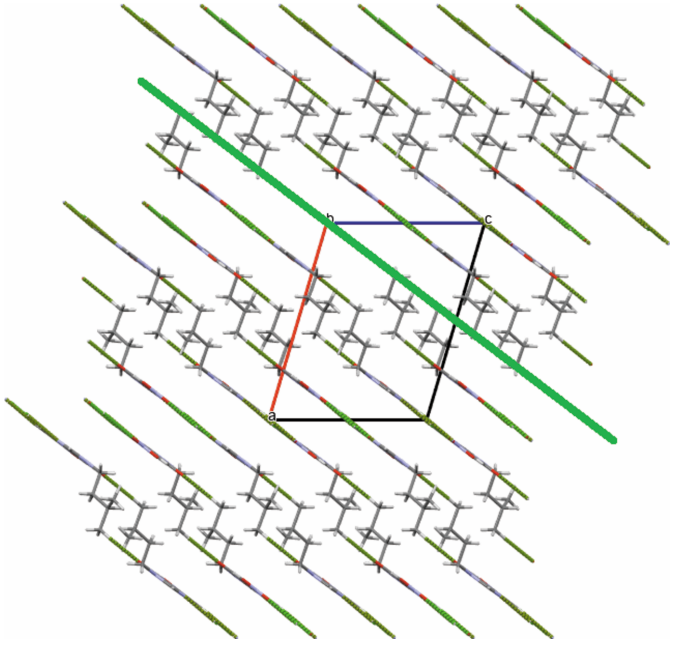


Figure 2
Crystal packing of (I) viewed along [010], showing intermolecular C—H···O and C—H···N contacts (green lines). The thick green line indicates the projected trace of a hydrogen-bonded layer parallel to ($\bar{2}$01).

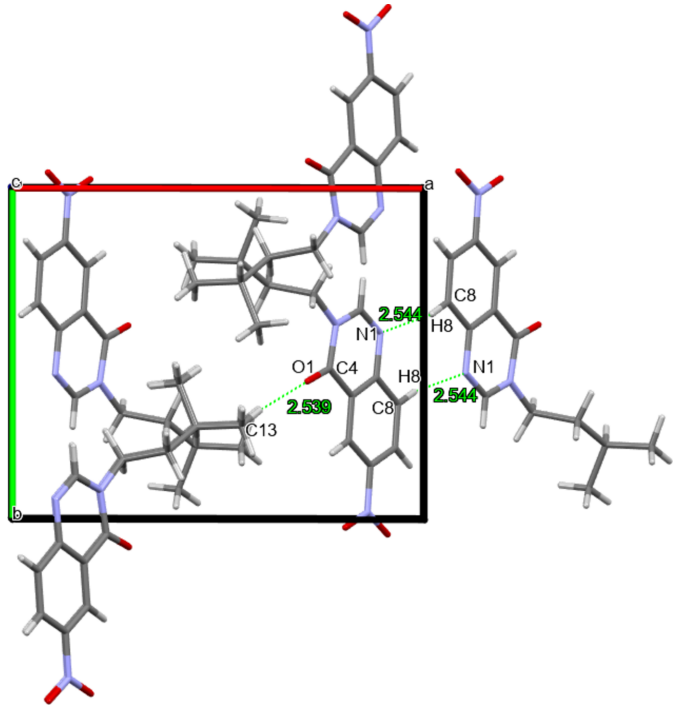


Figure 3
Detail of the packing with intermolecular C—H···O and C—H···N contacts indicated by green dashed lines.

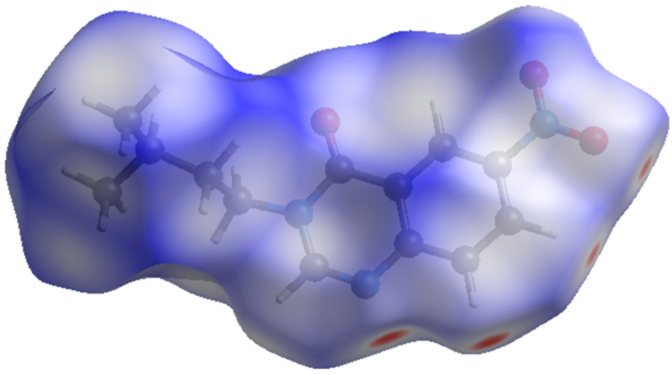


Figure 4
Hirshfeld surface of (I) mapped over d_{norm}.

the most abundant contributions are shown in Fig. 5. The highest contributions to the Hirshfeld surface arise from H···H contacts at 39.2%, followed by O···H/H···O, C···H/H···C and N···H/H···N interactions with contributions of 28.4%, 16.0% and 7.5% respectively. Minor contributors not shown in Fig. 5 are from C···O/O···C (4.3%), N···O/O···N (2.1%), N···C/C···N (1.1%), N···N (0.8%), O···O (0.3%) and C···C (0.3%) interactions.

5. Database survey

A search of the Cambridge Structural Database (CSD, version 2025.3.1; Groom *et al.*, 2016) identifies related quinazolin-4-one structures with refcodes JOJWOY (Zhang *et al.*, 2024), AFEWIT (Al-Suwaidan *et al.*, 2013), BOTMUT (Samarov *et al.*, 2009), DUVFEH (Gnanasekaran *et al.*, 2015), EVECEQ (Tojiboev *et al.*, 2025), GABHEZ (Elmuradov *et al.*, 2016), GAPPUK (Yu, 2012), QOQGOW (Davlatboyev *et al.*, 2024), PUFMAI (Davlatboyev *et al.*, 2025), AWABUY (El-Azab *et al.*, 2021), and RUGKEK (Wu *et al.*, 2009). For compounds with a nitro group attached to the ring system differences of the orientations of the nitro groups relative to compound (I) are found. In JOJWOY (2-amino-6,8-dinitroquinazolin-4-one hydrate), the O3—N1—C1—C2 torsion angle is 59.1 (9)°, while the O2—N4—C6—C7 torsion angle in (I) is 1.3 (2)°; in RUGKEK (7-fluoro-6-nitroquinazolin-4(3*H*)-one), the comparable torsion angle O3—N3—C5—C4 is −12.3 (3)°. The more extensively fused analogue DUVFEH (6-acetyl-2-nitrobenzo[4,5]imidazo-[2,1-*b*]quinazolin-12(6*H*)-one) has an O3—N4—C7—C8 torsion angle of −4.0 (11)°. In comparison, the O2—N4—C6—C7 torsion angle in the title compound is 1.3 (2)°, indicating that its nitro substituent is nearly coplanar with the quinazolinone aromatic ring. Because the compared compounds differ in their substitution patterns, these values describe local nitro-group conformations rather than an identical four-atom fragment in every case.

The N3-bound isoamyl substituent in compound (I) has an extended conformation. This flexible branched chain differs from the 2,3-pentamethylene unit in BOTMUT (6,8-dinitro-2,3-pentamethylene-3,4-dihydroquinazolin-4-one), in which the aliphatic segment is incorporated into a cyclic framework. A further structurally distinct example is AFEWIT {methyl 3-[(6-nitro-4-oxo-3-phenyl-3,4-dihydroquinazolin-2-yl)sulfanyl]-propanoate}, which contains an ester-bearing aliphatic substituent attached at the sulfur atom.

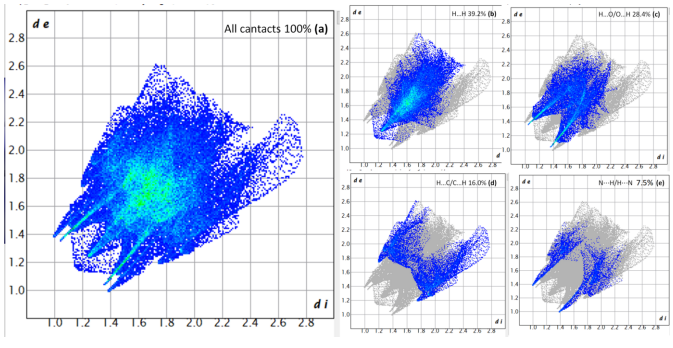


Figure 5
Two-dimensional fingerprint plots for the title compound, showing (*a*) all interactions, and decomposed into (*b*) H···H, (*c*) O···H/H···O, (*d*) C···H/H···C, (*e*) N···H/H···N interactions. Values for d_i and d_e represent the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

6. Synthesis and crystallization

Synthesis of 3-isoamylquinazolin-4-one. 1.46 g (0.01 mol) of quinazolin-4-one, 30 ml of ethyl alcohol (C_2H_5OH) and 0.672 g (0.012 mol) of KOH were placed into a 100 ml round-bottomed flask and mixed. Then 1.4 ml (1.6 g, d = 0.87 g ml^{-1}; 0.015 mol) of isoamyl chloride ($C_5H_{11}Cl$) was added to the cooled reaction mixture and heated at 348–353 K for 9 h. After cooling, 30 ml of 5%$_{wt}$ NaOH aqueous solution was added, and 70 ml of chloroform was poured into the solution for extraction, which resulted in 1.9 g of the intermediate (yield: 88%); melting point 338–340 K, R_f = 0.68 (benzene: acetone – 3:1).

Synthesis of 3-isoamyl-6-nitroquinazolin-4-one, (I). 20 ml of concentrated sulfuric acid were placed in a round-bottomed flask, cooled and connected to a magnetic stirrer (200 rotations per minute). Then 3-iso-amylquinazolin-4-one 2.16 g (0.01 mol) was added and dissolved. Sulfuric acid (0.005 mol) and nitric acid (0.005 mol) were mixed in a flask, cooled and dripped onto the solution with a dropping funnel (200 drops per minute). After complete addition, the mixture was heated at 313–315 K for 2 h and then placed in a refrigerator overnight. The mixture was then neutralized (pH 7), and the resulting precipitate filtered off. Colourless crystals suitable for X-ray diffraction analysis were recrystallized from ethanol; yield 91%.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms bonded to carbon were positioned geometrically and refined using a riding model with

U_{iso}(H) = 1.2U_{eq}(C) for CH and CH_2 groups and 1.5U_{eq}(C) for methyl groups. The latter were treated as rotating groups.

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Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{13}H_{15}N_3O_3$
M_r	261.28
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, b, c (Å)	13.3282 (9), 10.2832 (6), 10.2474 (6)
β (°)	106.416 (7)
V (Å^3)	1347.21 (15)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.78
Crystal size (mm)	0.20 × 0.15 × 0.05
Data collection	
Diffractometer	XtaLAB Synergy, Single source at home/near, HyPix3000
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2020)
T_{min}, T_{max}	0.239, 1.000
No. of measured, independent and observed [$I \geq 2u(I)$] reflections	6643, 2640, 1718
R_{int}	0.037
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.616
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.059, 0.199, 1.01
No. of reflections	2613
No. of parameters	175
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.22, −0.19

Computer programs: *CrysAlis PRO* (Rigaku OD, 2020), *SHELXT* (Sheldrick, 2015), *OLEX2.refine* (Bourhis *et al.*, 2015), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

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Computing details

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Crystal data

$C_{13}H_{15}N_3O_3$
M_r = 261.28
Monoclinic, $P2_1/c$
a = 13.3282 (9) Å
b = 10.2832 (6) Å
c = 10.2474 (6) Å
β = 106.416 (7)°
V = 1347.21 (15) Å^3
Z = 4
$F(000)$ = 552.0
D_x = 1.288 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 1864 reflections
θ = 5.5–69.4°
μ = 0.78 mm^{-1}
T = 293 K
Prism, colourless
0.20 × 0.15 × 0.05 mm

Data collection

XtaLAB Synergy, Single source at home/near, HyPix3000 diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2020)
T_{min} = 0.239, T_{max} = 1.000
6643 measured reflections
2640 independent reflections
1718 reflections with $I \geq 2u(I)$
R_{int} = 0.037
θ_{max} = 71.7°, θ_{min} = 3.5°
h = −14→16
k = −12→12
l = −12→8

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.199
S = 1.01
2613 reflections
175 parameters
0 restraints
24 constraints
Primary atom site location: dual
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1092P)^2 + 0.0954P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.030
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O2	0.91337 (16)	1.04756 (17)	0.8360 (2)	0.0794 (6)
N3	0.78714 (14)	0.41230 (18)	0.57360 (18)	0.0551 (5)
N4	0.86433 (16)	0.98032 (19)	0.7405 (2)	0.0652 (6)
N1	0.89582 (15)	0.43903 (18)	0.79896 (19)	0.0609 (5)
O3	0.8103 (2)	1.02617 (19)	0.6352 (2)	0.1086 (9)
C6	0.87157 (17)	0.8389 (2)	0.7541 (2)	0.0537 (5)
C8A	0.88591 (16)	0.5727 (2)	0.7819 (2)	0.0508 (5)
C4A	0.82610 (15)	0.6284 (2)	0.6599 (2)	0.0493 (5)
C5	0.81855 (17)	0.7634 (2)	0.6464 (2)	0.0535 (5)
H5	0.77847 (17)	0.8012 (2)	0.5661 (2)	0.0642 (7)*
C4	0.77133 (17)	0.5454 (2)	0.5468 (2)	0.0547 (6)
C8	0.93880 (18)	0.6537 (2)	0.8895 (2)	0.0595 (6)
H8	0.97873 (18)	0.6174 (2)	0.9707 (2)	0.0714 (7)*
C9	0.73215 (18)	0.3191 (2)	0.4681 (2)	0.0635 (6)
H13a	0.72927 (18)	0.3537 (2)	0.3791 (2)	0.0761 (8)*
H13b	0.77093 (18)	0.2381 (2)	0.4798 (2)	0.0761 (8)*
C2	0.84695 (17)	0.3690 (2)	0.6965 (2)	0.0589 (6)
H2	0.85320 (17)	0.2793 (2)	0.7076 (2)	0.0706 (7)*
C7	0.93173 (18)	0.7863 (2)	0.8750 (2)	0.0584 (6)
H7	0.96708 (18)	0.8403 (2)	0.9460 (2)	0.0701 (7)*
C10	0.6228 (2)	0.2930 (3)	0.4754 (3)	0.0768 (8)
H23a	0.6269 (2)	0.2429 (3)	0.5569 (3)	0.0921 (10)*
H23b	0.5899 (2)	0.3755 (3)	0.4842 (3)	0.0921 (10)*
C11	0.5536 (2)	0.2207 (3)	0.3540 (3)	0.0913 (10)
H33	0.5521 (2)	0.2720 (3)	0.2729 (3)	0.1096 (12)*
C12	0.5951 (3)	0.0888 (4)	0.3342 (4)	0.1238 (14)
H4Ba	0.602 (2)	0.0371 (11)	0.4142 (13)	0.186 (2)*
H4Bb	0.5478 (13)	0.0471 (13)	0.257 (2)	0.186 (2)*
H4Bc	0.6624 (11)	0.0978 (4)	0.318 (3)	0.186 (2)*
C13	0.4431 (3)	0.2152 (6)	0.3640 (5)	0.150 (2)
H1a	0.4419 (6)	0.169 (4)	0.445 (3)	0.224 (3)*
H1b	0.4175 (13)	0.3020 (6)	0.368 (5)	0.224 (3)*
H1c	0.3995 (8)	0.171 (4)	0.286 (2)	0.224 (3)*
O1	0.71749 (14)	0.58364 (17)	0.43714 (17)	0.0741 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0929 (13)	0.0491 (10)	0.0934 (13)	−0.0111 (9)	0.0220 (10)	−0.0173 (9)
N3	0.0590 (10)	0.0429 (9)	0.0595 (10)	−0.0032 (8)	0.0107 (8)	−0.0035 (8)
N4	0.0720 (13)	0.0428 (11)	0.0775 (14)	−0.0003 (10)	0.0160 (11)	−0.0024 (10)
N1	0.0680 (12)	0.0428 (10)	0.0639 (11)	0.0022 (9)	0.0055 (9)	0.0045 (8)
O3	0.147 (2)	0.0465 (11)	0.1019 (16)	0.0072 (12)	−0.0144 (14)	0.0134 (11)
C6	0.0572 (12)	0.0377 (11)	0.0649 (13)	0.0006 (9)	0.0153 (10)	−0.0016 (10)
C8A	0.0507 (11)	0.0433 (11)	0.0560 (11)	0.0025 (9)	0.0111 (9)	0.0020 (9)

C4A	0.0487 (10)	0.0432 (11)	0.0531 (11)	0.0017 (9)	0.0099 (9)	0.0004 (9)
C5	0.0558 (12)	0.0449 (12)	0.0562 (12)	0.0031 (10)	0.0099 (10)	0.0032 (10)
C4	0.0567 (12)	0.0470 (12)	0.0558 (12)	−0.0011 (10)	0.0087 (10)	0.0007 (10)
C8	0.0636 (13)	0.0514 (14)	0.0555 (12)	0.0034 (11)	0.0039 (10)	0.0010 (10)
C9	0.0703 (15)	0.0511 (13)	0.0670 (14)	−0.0092 (11)	0.0162 (12)	−0.0098 (11)
C2	0.0619 (13)	0.0410 (11)	0.0693 (13)	0.0015 (11)	0.0116 (11)	0.0024 (11)
C7	0.0614 (13)	0.0516 (13)	0.0576 (12)	−0.0026 (10)	0.0092 (10)	−0.0092 (10)
C10	0.0765 (16)	0.083 (2)	0.0721 (16)	−0.0216 (15)	0.0237 (13)	−0.0174 (14)
C11	0.085 (2)	0.103 (2)	0.0822 (19)	−0.0324 (18)	0.0166 (15)	−0.0238 (18)
C12	0.143 (3)	0.100 (3)	0.123 (3)	−0.043 (2)	0.029 (2)	−0.041 (2)
C13	0.087 (2)	0.203 (6)	0.153 (4)	−0.056 (3)	0.025 (2)	−0.065 (4)
O1	0.0886 (12)	0.0598 (10)	0.0582 (9)	−0.0003 (9)	−0.0050 (8)	0.0018 (8)

Geometric parameters (Å, º)

O2—N4	1.225 (2)	C9—H13a	0.9700
N3—C4	1.400 (3)	C9—H13b	0.9700
N3—C9	1.475 (3)	C9—C10	1.504 (3)
N3—C2	1.361 (3)	C2—H2	0.9300
N4—O3	1.210 (3)	C7—H7	0.9300
N4—C6	1.462 (3)	C10—H23a	0.9700
N1—C8A	1.387 (3)	C10—H23b	0.9700
N1—C2	1.288 (3)	C10—C11	1.518 (4)
C6—C5	1.371 (3)	C11—H33	0.9800
C6—C7	1.382 (3)	C11—C12	1.500 (5)
C8A—C4A	1.401 (3)	C11—C13	1.507 (4)
C8A—C8	1.402 (3)	C12—H4Ba	0.9600
C4A—C5	1.395 (3)	C12—H4Bb	0.9600
C4A—C4	1.458 (3)	C12—H4Bc	0.9600
C5—H5	0.9300	C13—H1a	0.9600
C4—O1	1.215 (3)	C13—H1b	0.9600
C8—H8	0.9300	C13—H1c	0.9600
C8—C7	1.373 (3)		

C9—N3—C4	118.39 (18)	N1—C2—N3	126.9 (2)
C2—N3—C4	121.16 (19)	H2—C2—N3	116.54 (12)
C2—N3—C9	120.34 (19)	H2—C2—N1	116.54 (13)
O3—N4—O2	122.7 (2)	C8—C7—C6	119.3 (2)
C6—N4—O2	118.6 (2)	H7—C7—C6	120.33 (13)
C6—N4—O3	118.6 (2)	H7—C7—C8	120.33 (13)
C2—N1—C8A	116.30 (18)	H23a—C10—C9	108.57 (14)
C5—C6—N4	118.8 (2)	H23b—C10—C9	108.57 (15)
C7—C6—N4	118.7 (2)	H23b—C10—H23a	107.5
C7—C6—C5	122.5 (2)	C11—C10—C9	114.8 (2)
C4A—C8A—N1	121.83 (19)	C11—C10—H23a	108.57 (17)
C8—C8A—N1	118.74 (19)	C11—C10—H23b	108.57 (18)
C8—C8A—C4A	119.43 (19)	H33—C11—C10	107.02 (17)
C5—C4A—C8A	120.1 (2)	C12—C11—C10	113.1 (3)

C4—C4A—C8A	120.0 (2)	C12—C11—H33	107.0 (2)
C4—C4A—C5	119.82 (19)	C13—C11—C10	110.0 (3)
C4A—C5—C6	118.5 (2)	C13—C11—H33	107.0 (3)
H5—C5—C6	120.76 (13)	C13—C11—C12	112.4 (3)
H5—C5—C4A	120.76 (13)	H4Ba—C12—C11	109.5
C4A—C4—N3	113.75 (18)	H4Bb—C12—C11	109.5
O1—C4—N3	120.9 (2)	H4Bb—C12—H4Ba	109.5
O1—C4—C4A	125.3 (2)	H4Bc—C12—C11	109.5
H8—C8—C8A	119.94 (12)	H4Bc—C12—H4Ba	109.5
C7—C8—C8A	120.1 (2)	H4Bc—C12—H4Bb	109.5
C7—C8—H8	119.94 (13)	H1a—C13—C11	109.5
H13a—C9—N3	109.32 (12)	H1b—C13—C11	109.5
H13b—C9—N3	109.32 (12)	H1b—C13—H1a	109.5
H13b—C9—H13a	108.0	H1c—C13—C11	109.5
C10—C9—N3	111.54 (19)	H1c—C13—H1a	109.5
C10—C9—H13a	109.32 (14)	H1c—C13—H1b	109.5
C10—C9—H13b	109.32 (16)		

O2—N4—C6—C5	−178.7 (2)	N1—C8A—C4A—C4	0.6 (2)
O2—N4—C6—C7	1.3 (2)	N1—C8A—C8—C7	179.1 (2)
N3—C4—C4A—C8A	−1.2 (2)	C6—C5—C4A—C8A	0.7 (2)
N3—C4—C4A—C5	178.99 (18)	C6—C5—C4A—C4	−179.5 (2)
N3—C9—C10—C11	168.0 (2)	C6—C7—C8—C8A	0.4 (3)
N3—C2—N1—C8A	0.2 (3)	C8A—C4A—C4—O1	179.9 (2)
N4—C6—C5—C4A	179.8 (2)	C9—C10—C11—C12	60.6 (3)
N4—C6—C7—C8	179.7 (2)	C9—C10—C11—C13	−172.9 (4)
N1—C8A—C4A—C5	−179.6 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H1*c*···O1^{i}	0.96 (3)	2.54 (2)	3.493 (5)	172 (3)
C8—H8···N1^{ii}	0.93 (1)	2.54 (1)	3.462 (3)	169 (1)

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