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Synthesis and crystal structure of 3-(2-{3-[2-(2-oxooxazolidin-3-yl)ethoxy]quinoxalin-2-yloxy}-ethyl)oxazolidin-2-one

Fatima Ezzahra Aboutofil,[a] Nour El Hoda Mustaphi,[a]* Olivier Blacque,[b] Tuncer Hökelek,[c] Ahmed Mazzah,[d] Lhoussaine El Ghayati[a] and Nada Kheira Sebbar[e,f]

[a]Laboratory of Heterocyclic Organic Chemistry, Medicines Science Research, Center, Pharmacochemistry Competence Center, Mohammed V University in Rabat, Faculté des Sciences, Av. Ibn Battouta, BP 1014, Rabat, Morocco, [b]University of Zurich, Department of Chemistry, Winterthurerstrasse 190, CH-8057 Zurich, Switzerland, [c]Department of Physics, Hacettepe University, 06800 Beytepe, Ankara, Türkiye, [d]Science and Technology of Lille USR 3290, Villeneuve d'ascq cedex, France, [e]Laboratory of Organic and Physical Chemistry, Applied Bioorganic Chemistry Team, Faculty of Sciences, Ibnou Zohr University, Agadir, Morocco, and [f]Laboratory of Plant Chemistry, Organic and Bioorganic Synthesis, Faculty of Sciences, Mohammed V University in Rabat, 4 Avenue Ibn Battouta BP 1014 RP., Rabat, Morocco. *Correspondence e-mail: nourelhoda.mustaphi@fsr.um5.ac.ma

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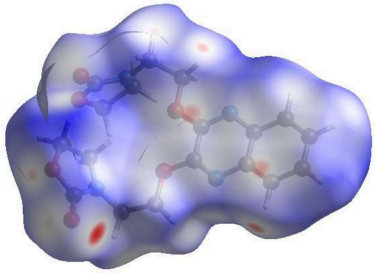
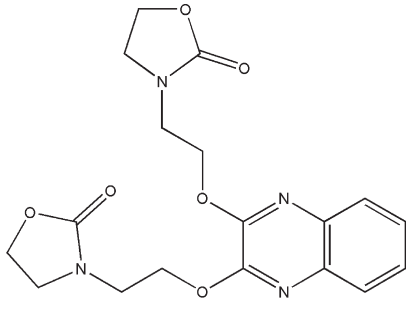
In the title compound, $C_{18}H_{20}N_4O_6$, one of the oxazolidine rings adopts a twisted conformation and the other is a shallow envelope. In the crystal, weak C—H···O hydrogen bonds and π–π stacking interactions help to consolidate a three-dimensional architecture. The Hirshfeld surface analysis of the crystal structure indicates that the most important contributions for the crystal packing are from H···H (48.4%) and H···O/O···H (29.1%) contacts.

1. Chemical context

Quinoxaline and its derivatives are widely used in various fields, including medicine (Kaushal *et al.*, 2019; Montana *et al.*, 2019), pharmacology, molecular biology, neuroscience, immunology, microbiology, agriculture, chemistry, toxicology, materials science, and biochemistry (Balderas-Renteria *et al.*, 2012; Pereira *et al.*, 2015; Zeb *et al.*, 2014; Tangherlini *et al.*, 2019; Vieira *et al.*, 2014; Zheng *et al.*, 2002).

The quinoxaline molecule has been utilized as a precursor for synthesizing bioactive derivatives, with several research teams emphasizing its potential applications in the pharmaceutical and therapeutic fields (Raoa *et al.*, 2010; Yousra *et al.*, 2023). Different synthesis methodologies have been detailed in the literature, reflecting extensive research efforts to elucidate these compounds' properties and applications (*e.g.*, Gu *et al.*, 2017). Building on our previous research into the synthesis of quinoxaline derivatives (Yousra *et al.*, 2023), we have synthesized the title compound, $C_{18}H_{20}N_4O_6$ (**I**), and we now describe its synthesis, crystal structure and Hirshfeld surface.





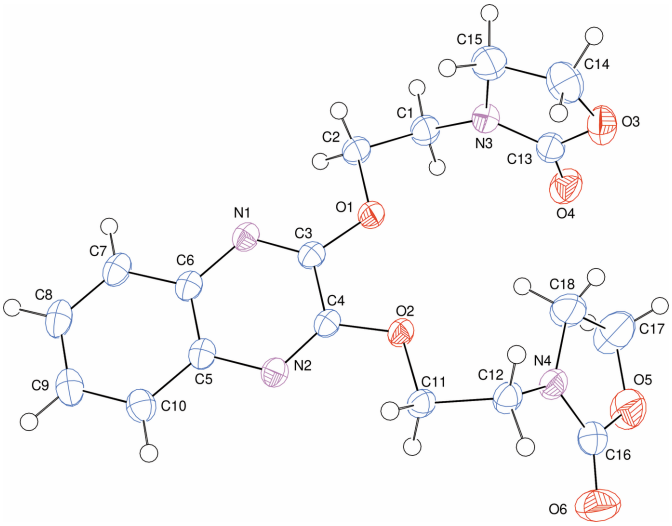


Figure 1
The molecular structure of the title molecule with 50% probability ellipsoids.

2. Structural commentary

Compound (**I**) contains an almost planar quinoxaline fused ring and two oxazolidine rings (Fig. 1), where the oxazolidine (*C*, N3/O3/C13–C15) and (*D*, N4/O5/C16–C18) rings are in half-chair [with a puckering parameter value of $\varphi = 305.0\ (4)^\circ$] and shallow envelope conformations, respectively. In ring *D*, atom N4 is at the flap position and is 0.0849 (11) Å away from the best least-squares plane of the other four atoms. The almost planar *A* (N1/N2/C3–C6) and *B* (C5–C10) rings are oriented at a dihedral angle of 1.46 (4)°. Atoms O1, O2 and C11 are −0.094 (1), 0.059 (1) and 0.070 (1) Å, respectively, away from the best least-squares plane of ring *A*. The side chains both have *anti–gauche* conformations as indicated by the following torsion angles: C3—O1—C2—C1 = −162.00 (10), O1—C2—C1—N3 = −55.36 (14), C4—O2—C11—C12 = −174.35 (9) and O2—C11—C12—N4 = −57.76 (13)°. The dihedral angles between the quinoxaline ring and the pendant oxazolidine *C* and *D* rings (all atoms) are 85.72 (6) and 56.91 (7)°, respectively; the equivalent angle between the oxazolidine rings is 89.98 (9)°.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14*A*···O6^{i}	0.99	2.37	3.189 (2)	140
C10—H10···O5^{ii}	0.95	2.56	3.4935 (18)	168

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

3. Supramolecular features

In the crystal structure of (**I**), the molecules are linked by C—H···O hydrogen bonds (Table 1 and Fig. 2). Aromatic π–π stacking interactions between the quinoxaline *A* and *B* rings of adjacent molecules with a shortest intercentroid distance of 3.5155 (7) Å may help to consolidate the packing. No C—H···π interactions could be identified.

4. Hirshfeld surface analysis

A Hirshfeld surface (HS) analysis was carried out using *Crystal Explorer 17.5* (Spackman *et al.*, 2021) to investigate the intermolecular interactions in the crystal of (**I**). The HS is shown in Fig. 3, where the bright-red spots correspond to the respective donors and/or acceptors. According to the two-dimensional fingerprint plots (McKinnon *et al.*, 2007), the intermolecular H···H and H···O/O···H contacts make the most important contributions to the HS of 48.4% and 29.1%, respectively (Fig. 4). All other contact types contribute 5% or less to the surface.

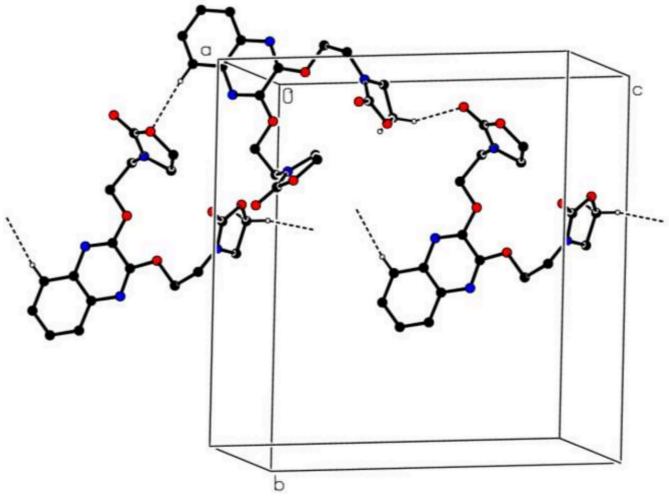


Figure 2
A partial packing diagram viewed down the *a*-axis direction. Intermolecular C—H···O hydrogen bonds are shown as dashed lines. H atoms not involved in these interactions are omitted for clarity.

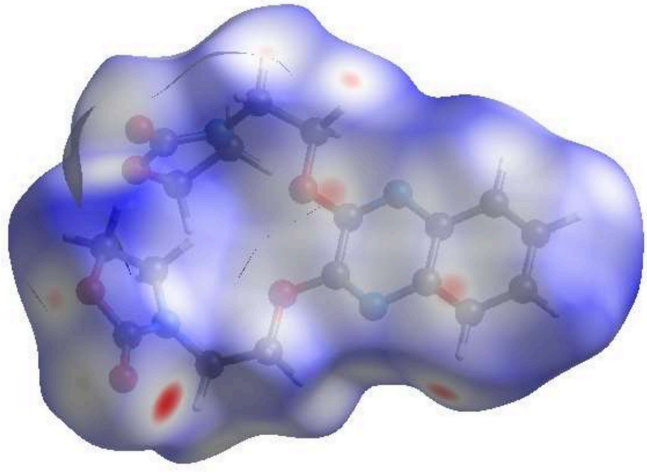


Figure 3
View of the three-dimensional Hirshfeld surface of the title compound plotted over d_{norm}.

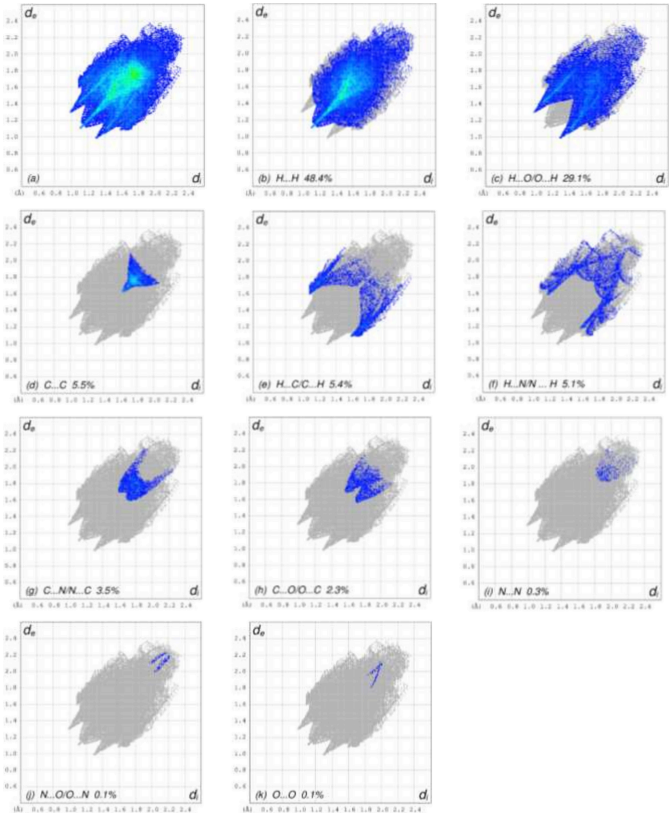


Figure 4
The full two-dimensional fingerprint plots for the title compound, showing (*a*) all interactions, and delineated into (*b*) H···H, (*c*) H···O/O···H, (*d*) C···C, (*e*) H···C/C···H, (*f*) H···N/N···H, (*g*) C···N/N···C, (*h*) C···O/O···C, (i) N···N, (*j*) N···O/O···N and (*k*) O···O interactions. The d_i and d_e values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

5. Database survey

A search of the Cambridge Structural Database (CSD) (Groom *et al.*, 2016; updated to January 2024) using the search fragment (**II**) yielded 25 hits of which those most similar to the title molecule have the formula (**III**) with R = Me and R' = CH_2CO_2H (CSD refcode DEZJAW; Missioui *et al.*, 2018) or benzyl (DUSHUV; Ramli *et al.*, 2010) with R = CF_3 and R' = *i*-Bu (DUBPUO; Wei *et al.*, 2019), with R = Ph and R' = CH_2 (cyclo-$CHCH_2O$) and R' = benzyl (PUGGII; Benzeid *et al.*, 2009). As expected, in all these hits, the dihydroquinoxaline ring system is essentially planar with the dihedral angle between the constituent rings being less than 1° or having the nitrogen atom bearing the exocyclic substituent less than 0.03 Å from the mean plane of the remaining nine atoms.

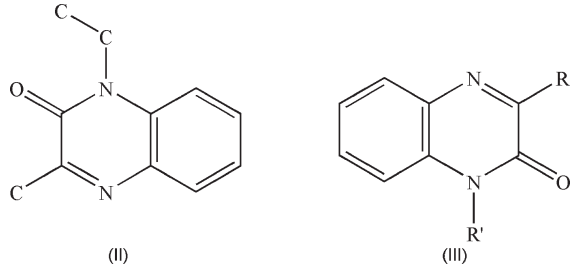


Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{20}N_4O_6$
M_r	388.38
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	160
a, b, c (Å)	6.6576 (1), 17.1463 (2), 15.8105 (2)
β (°)	98.935 (1)
V (Å^3)	1782.92 (4)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.93
Crystal size (mm)	0.25 × 0.21 × 0.10
Data collection	
Diffractometer	XtaLAB Synergy, Dualflex, HyPix
Absorption correction	Analytical (*CrysAlis PRO*; Rigaku OD, 2024)
T_{min}, T_{max}	0.845, 0.932
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	23056, 3781, 3577
R_{int}	0.027
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.633
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.038, 0.099, 1.06
No. of reflections	3781
No. of parameters	254
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.35, −0.29

Computer programs: *CrysAlis PRO* (Rigaku OD, 2024), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2019/3* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

6. Synthesis and crystallization

A solution of quinoxaline-2,3-dione (0.29 g, 1.00 mmol) in dimethylformamide (15 ml) was prepared. To this solution, tetra-*n*-butylammonium bromide (0.1 mmol), 2.2 equivalents of bis(2-chloroethyl)amine hydrochloride, and 2.00 equivalents of potassium carbonate were added. The mixture was stirred at 353 K for 6 h. After stirring, the salts were removed by filtration, and the solution was evaporated under reduced pressure. The resulting residue was dissolved in dichloromethane. The remaining salts were extracted with distilled water. The mixture obtained was then chromatographed on a silica gel column using an eluent of ethyl acetate and hexane in a 4:1 ratio. The solid isolate was recrystallized from an ethanol solution, resulting in crystals of (**I**) with a yield of 56%.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The C-bound hydrogen-atom positions were calculated geometrically at distances of 0.95 Å (for aromatic CH) and 0.99 Å (for CH_2) and they were refined using a riding model by applying the constraint U_{iso}(H) = 1.2U_{eq}(C).

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supporting information

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Synthesis and crystal structure of 3-(2-{3-[2-(2-oxooxazolidin-3-yl)ethoxy]-quinoxalin-2-yloxy}ethyl)oxazolidin-2-one

Fatima Ezzahra Aboutofil, Nour El Hoda Mustaphi, Olivier Blacque, Tuncer Hökelek, Ahmed Mazzah, Lhoussaine El Ghayati and Nada Kheira Sebbar

Computing details

3-(2-{3-[2-(2-Oxooxazolidin-3-yl)ethoxy]quinoxalin-2-yloxy}ethyl)oxazolidin-2-one

Crystal data

$C_{18}H_{20}N_4O_6$
$M_r = 388.38$
Monoclinic, $P2_1/n$
$a = 6.6576$ (1) Å
$b = 17.1463$ (2) Å
$c = 15.8105$ (2) Å
$\beta = 98.935$ (1)°
$V = 1782.92$ (4) Å^3
$Z = 4$
$F(000) = 816$
$D_x = 1.447$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 17516 reflections
$\theta = 3.8$–$79.5°$
$\mu = 0.93$ mm^{-1}
$T = 160$ K
Plate, colourless
0.25 × 0.21 × 0.10 mm

Data collection

XtaLAB Synergy, Dualflex, HyPix 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: analytical (CrysAlisPro; Rigaku OD, 2024)
$T_{min} = 0.845$, $T_{max} = 0.932$
23056 measured reflections
3781 independent reflections
3577 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 77.4°$, $\theta_{min} = 3.8°$
$h = -8 \rightarrow 8$
$k = -21 \rightarrow 21$
$l = -17 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.099$
$S = 1.06$
3781 reflections
254 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0447P)^2 + 0.6483P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}
Extinction correction: *SHELXL2019/3* (Sheldrick, 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0023 (2)

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.34531 (13)	0.47199 (5)	0.72202 (5)	0.02841 (19)
O2	0.29395 (12)	0.35049 (4)	0.62370 (5)	0.02608 (19)
O3	0.35795 (16)	0.33324 (6)	0.96229 (7)	0.0444 (3)
O4	0.66392 (15)	0.37070 (6)	0.93404 (7)	0.0451 (3)
O5	0.74284 (18)	0.16514 (7)	0.76528 (7)	0.0527 (3)
O6	0.62002 (19)	0.11202 (8)	0.63787 (7)	0.0587 (3)
N1	0.28423 (15)	0.55758 (6)	0.60819 (6)	0.0269 (2)
N2	0.25336 (14)	0.42434 (6)	0.50000 (6)	0.0253 (2)
N3	0.37902 (16)	0.44689 (6)	0.89855 (7)	0.0322 (2)
N4	0.44993 (17)	0.20867 (6)	0.69704 (7)	0.0331 (2)
C1	0.4760 (2)	0.51244 (7)	0.86354 (8)	0.0342 (3)
H1A	0.616539	0.497667	0.857060	0.041*
H1B	0.484189	0.556502	0.904393	0.041*
C2	0.3645 (2)	0.53887 (7)	0.77796 (8)	0.0328 (3)
H2A	0.228380	0.559210	0.784233	0.039*
H2B	0.441442	0.580793	0.754216	0.039*
C3	0.30273 (16)	0.48736 (7)	0.63769 (7)	0.0252 (2)
C4	0.28227 (16)	0.41917 (6)	0.58255 (7)	0.0241 (2)
C5	0.23938 (16)	0.49903 (7)	0.46633 (8)	0.0261 (2)
C6	0.25158 (16)	0.56504 (7)	0.51985 (8)	0.0266 (2)
C7	0.23349 (18)	0.64004 (7)	0.48354 (9)	0.0316 (3)
H7	0.240283	0.684707	0.519426	0.038*
C8	0.20594 (18)	0.64869 (8)	0.39597 (9)	0.0354 (3)
H8	0.193559	0.699445	0.371627	0.043*
C9	0.19602 (19)	0.58335 (8)	0.34250 (9)	0.0358 (3)
H9	0.178341	0.590080	0.282161	0.043*
C10	0.21172 (18)	0.50923 (8)	0.37678 (8)	0.0314 (3)
H10	0.203901	0.465090	0.340091	0.038*
C11	0.27737 (18)	0.28136 (6)	0.57133 (7)	0.0266 (2)
H11A	0.395000	0.277258	0.540209	0.032*
H11B	0.151217	0.282899	0.528962	0.032*
C12	0.27329 (19)	0.21297 (7)	0.63101 (8)	0.0298 (3)
H12A	0.149795	0.216567	0.658525	0.036*
H12B	0.263947	0.164211	0.597081	0.036*
C13	0.4844 (2)	0.38405 (7)	0.93076 (8)	0.0335 (3)
C14	0.1517 (2)	0.36156 (10)	0.94072 (11)	0.0483 (4)
H14A	0.077858	0.356549	0.990193	0.058*
H14B	0.077252	0.332043	0.891836	0.058*
C15	0.1730 (2)	0.44643 (9)	0.91721 (10)	0.0429 (3)

H15A	0.073565	0.461243	0.866518	0.051*
H15B	0.157556	0.481479	0.965547	0.051*
C16	0.6022 (2)	0.15857 (8)	0.69375 (8)	0.0366 (3)
C17	0.6778 (4)	0.22219 (12)	0.82074 (12)	0.0720 (6)
H17A	0.773792	0.266660	0.828125	0.086*
H17B	0.670734	0.199276	0.877681	0.086*
C18	0.4690 (3)	0.24899 (9)	0.77867 (9)	0.0520 (4)
H18A	0.361999	0.232637	0.811984	0.062*
H18B	0.463720	0.306297	0.771004	0.062*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0383 (5)	0.0205 (4)	0.0264 (4)	0.0002 (3)	0.0047 (3)	−0.0015 (3)
O2	0.0325 (4)	0.0185 (4)	0.0268 (4)	0.0001 (3)	0.0032 (3)	0.0000 (3)
O3	0.0531 (6)	0.0357 (5)	0.0436 (5)	−0.0012 (4)	0.0054 (4)	0.0096 (4)
O4	0.0414 (6)	0.0437 (6)	0.0480 (6)	0.0111 (4)	−0.0001 (4)	0.0032 (5)
O5	0.0546 (7)	0.0533 (6)	0.0442 (6)	0.0125 (5)	−0.0111 (5)	0.0030 (5)
O6	0.0615 (7)	0.0665 (8)	0.0468 (6)	0.0281 (6)	0.0044 (5)	−0.0123 (6)
N1	0.0261 (5)	0.0223 (5)	0.0326 (5)	0.0002 (4)	0.0051 (4)	0.0015 (4)
N2	0.0236 (5)	0.0241 (5)	0.0280 (5)	0.0001 (3)	0.0028 (4)	0.0012 (4)
N3	0.0364 (6)	0.0299 (5)	0.0304 (5)	0.0043 (4)	0.0053 (4)	0.0020 (4)
N4	0.0451 (6)	0.0238 (5)	0.0285 (5)	0.0043 (4)	−0.0010 (4)	−0.0016 (4)
C1	0.0425 (7)	0.0263 (6)	0.0330 (6)	−0.0020 (5)	0.0034 (5)	−0.0029 (5)
C2	0.0464 (7)	0.0216 (5)	0.0300 (6)	0.0009 (5)	0.0051 (5)	−0.0039 (5)
C3	0.0233 (5)	0.0232 (5)	0.0295 (6)	0.0001 (4)	0.0054 (4)	0.0003 (4)
C4	0.0220 (5)	0.0207 (5)	0.0297 (6)	0.0002 (4)	0.0047 (4)	0.0011 (4)
C5	0.0202 (5)	0.0262 (6)	0.0318 (6)	−0.0001 (4)	0.0042 (4)	0.0044 (4)
C6	0.0204 (5)	0.0255 (6)	0.0342 (6)	0.0005 (4)	0.0053 (4)	0.0042 (4)
C7	0.0263 (6)	0.0252 (6)	0.0436 (7)	0.0005 (4)	0.0061 (5)	0.0059 (5)
C8	0.0275 (6)	0.0324 (6)	0.0464 (7)	0.0019 (5)	0.0057 (5)	0.0153 (5)
C9	0.0300 (6)	0.0417 (7)	0.0354 (6)	0.0012 (5)	0.0042 (5)	0.0130 (5)
C10	0.0281 (6)	0.0348 (6)	0.0310 (6)	−0.0006 (5)	0.0032 (5)	0.0040 (5)
C11	0.0305 (6)	0.0205 (5)	0.0280 (5)	−0.0003 (4)	0.0024 (4)	−0.0025 (4)
C12	0.0343 (6)	0.0217 (5)	0.0328 (6)	−0.0017 (4)	0.0032 (5)	−0.0002 (4)
C13	0.0436 (7)	0.0298 (6)	0.0257 (6)	0.0017 (5)	0.0007 (5)	−0.0019 (5)
C14	0.0453 (8)	0.0538 (9)	0.0464 (8)	−0.0081 (7)	0.0084 (6)	0.0063 (7)
C15	0.0377 (7)	0.0479 (8)	0.0438 (8)	0.0052 (6)	0.0090 (6)	0.0029 (6)
C16	0.0415 (7)	0.0344 (7)	0.0331 (6)	0.0043 (5)	0.0033 (5)	0.0041 (5)
C17	0.1003 (15)	0.0538 (10)	0.0487 (9)	0.0250 (10)	−0.0297 (10)	−0.0142 (8)
C18	0.0775 (11)	0.0436 (8)	0.0309 (7)	0.0155 (8)	−0.0045 (7)	−0.0085 (6)

Geometric parameters (Å, º)

O1—C2	1.4416 (14)	C5—C6	1.4079 (17)
O1—C3	1.3454 (14)	C5—C10	1.4100 (17)
O2—C4	1.3418 (13)	C6—C7	1.4057 (16)
O2—C11	1.4403 (13)	C7—H7	0.9500

O3—C13	1.3589 (17)	C7—C8	1.3762 (19)
O3—C14	1.447 (2)	C8—H8	0.9500
O4—C13	1.2101 (17)	C8—C9	1.399 (2)
O5—C16	1.3563 (17)	C9—H9	0.9500
O5—C17	1.425 (2)	C9—C10	1.3792 (18)
O6—C16	1.2100 (18)	C10—H10	0.9500
N1—C3	1.2901 (15)	C11—H11A	0.9900
N1—C6	1.3857 (16)	C11—H11B	0.9900
N2—C4	1.2924 (15)	C11—C12	1.5080 (16)
N2—C5	1.3846 (15)	C12—H12A	0.9900
N3—C1	1.4483 (17)	C12—H12B	0.9900
N3—C13	1.3421 (16)	C14—H14A	0.9900
N3—C15	1.4474 (18)	C14—H14B	0.9900
N4—C12	1.4480 (16)	C14—C15	1.514 (2)
N4—C16	1.3359 (17)	C15—H15A	0.9900
N4—C18	1.4522 (17)	C15—H15B	0.9900
C1—H1A	0.9900	C17—H17A	0.9900
C1—H1B	0.9900	C17—H17B	0.9900
C1—C2	1.5084 (18)	C17—C18	1.516 (3)
C2—H2A	0.9900	C18—H18A	0.9900
C2—H2B	0.9900	C18—H18B	0.9900
C3—C4	1.4521 (15)		

C3—O1—C2	115.92 (9)	C5—C10—H10	120.0
C4—O2—C11	116.75 (9)	C9—C10—C5	119.93 (12)
C13—O3—C14	108.53 (11)	C9—C10—H10	120.0
C16—O5—C17	109.50 (12)	O2—C11—H11A	110.4
C3—N1—C6	116.22 (10)	O2—C11—H11B	110.4
C4—N2—C5	116.25 (10)	O2—C11—C12	106.71 (9)
C13—N3—C1	122.03 (11)	H11A—C11—H11B	108.6
C13—N3—C15	111.99 (11)	C12—C11—H11A	110.4
C15—N3—C1	125.10 (11)	C12—C11—H11B	110.4
C12—N4—C18	124.44 (11)	N4—C12—C11	113.52 (10)
C16—N4—C12	122.74 (11)	N4—C12—H12A	108.9
C16—N4—C18	112.25 (11)	N4—C12—H12B	108.9
N3—C1—H1A	109.0	C11—C12—H12A	108.9
N3—C1—H1B	109.0	C11—C12—H12B	108.9
N3—C1—C2	112.93 (11)	H12A—C12—H12B	107.7
H1A—C1—H1B	107.8	O4—C13—O3	121.80 (12)
C2—C1—H1A	109.0	O4—C13—N3	128.51 (13)
C2—C1—H1B	109.0	N3—C13—O3	109.68 (12)
O1—C2—C1	107.19 (10)	O3—C14—H14A	110.7
O1—C2—H2A	110.3	O3—C14—H14B	110.7
O1—C2—H2B	110.3	O3—C14—C15	105.00 (12)
C1—C2—H2A	110.3	H14A—C14—H14B	108.8
C1—C2—H2B	110.3	C15—C14—H14A	110.7
H2A—C2—H2B	108.5	C15—C14—H14B	110.7
O1—C3—C4	115.02 (10)	N3—C15—C14	100.55 (11)

N1—C3—O1	122.32 (10)	N3—C15—H15A	111.7
N1—C3—C4	122.65 (11)	N3—C15—H15B	111.7
O2—C4—C3	115.00 (10)	C14—C15—H15A	111.7
N2—C4—O2	122.56 (10)	C14—C15—H15B	111.7
N2—C4—C3	122.44 (10)	H15A—C15—H15B	109.4
N2—C5—C6	121.22 (10)	O6—C16—O5	122.03 (13)
N2—C5—C10	119.43 (11)	O6—C16—N4	127.85 (13)
C6—C5—C10	119.35 (11)	N4—C16—O5	110.11 (12)
N1—C6—C5	121.12 (10)	O5—C17—H17A	110.4
N1—C6—C7	119.09 (11)	O5—C17—H17B	110.4
C7—C6—C5	119.78 (11)	O5—C17—C18	106.47 (13)
C6—C7—H7	120.0	H17A—C17—H17B	108.6
C8—C7—C6	119.93 (12)	C18—C17—H17A	110.4
C8—C7—H7	120.0	C18—C17—H17B	110.4
C7—C8—H8	119.7	N4—C18—C17	101.14 (13)
C7—C8—C9	120.54 (11)	N4—C18—H18A	111.5
C9—C8—H8	119.7	N4—C18—H18B	111.5
C8—C9—H9	119.8	C17—C18—H18A	111.5
C10—C9—C8	120.46 (12)	C17—C18—H18B	111.5
C10—C9—H9	119.8	H18A—C18—H18B	109.4

O1—C3—C4—O2	4.66 (14)	C6—C5—C10—C9	−0.28 (17)
O1—C3—C4—N2	−175.86 (10)	C6—C7—C8—C9	−0.10 (18)
O2—C11—C12—N4	−57.76 (13)	C7—C8—C9—C10	0.64 (19)
O3—C14—C15—N3	19.93 (15)	C8—C9—C10—C5	−0.44 (19)
O5—C17—C18—N4	−6.2 (2)	C10—C5—C6—N1	−178.23 (10)
N1—C3—C4—O2	−176.22 (10)	C10—C5—C6—C7	0.82 (16)
N1—C3—C4—N2	3.25 (18)	C11—O2—C4—N2	1.41 (15)
N1—C6—C7—C8	178.43 (10)	C11—O2—C4—C3	−179.12 (9)
N2—C5—C6—N1	1.99 (16)	C12—N4—C16—O5	−177.58 (11)
N2—C5—C6—C7	−178.96 (10)	C12—N4—C16—O6	1.4 (2)
N2—C5—C10—C9	179.50 (11)	C12—N4—C18—C17	178.95 (14)
N3—C1—C2—O1	−55.36 (14)	C13—O3—C14—C15	−17.07 (15)
C1—N3—C13—O3	177.45 (11)	C13—N3—C1—C2	132.78 (12)
C1—N3—C13—O4	−2.1 (2)	C13—N3—C15—C14	−17.38 (15)
C1—N3—C15—C14	173.26 (12)	C14—O3—C13—O4	−173.94 (13)
C2—O1—C3—N1	1.41 (16)	C14—O3—C13—N3	6.47 (15)
C2—O1—C3—C4	−179.46 (10)	C15—N3—C1—C2	−58.87 (16)
C3—O1—C2—C1	−162.00 (10)	C15—N3—C13—O3	7.71 (15)
C3—N1—C6—C5	0.10 (16)	C15—N3—C13—O4	−171.84 (14)
C3—N1—C6—C7	−178.95 (10)	C16—O5—C17—C18	3.4 (2)
C4—O2—C11—C12	−174.35 (9)	C16—N4—C12—C11	−102.91 (14)
C4—N2—C5—C6	−1.41 (16)	C16—N4—C18—C17	7.40 (18)
C4—N2—C5—C10	178.81 (10)	C17—O5—C16—O6	−177.74 (17)
C5—N2—C4—O2	178.41 (9)	C17—O5—C16—N4	1.34 (19)
C5—N2—C4—C3	−1.03 (16)	C18—N4—C12—C11	86.40 (16)
C5—C6—C7—C8	−0.63 (17)	C18—N4—C16—O5	−5.86 (17)
C6—N1—C3—O1	176.48 (9)	C18—N4—C16—O6	173.16 (16)

C6—N1—C3—C4	−2.57 (16)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14*A*···O6^{i}	0.99	2.37	3.189 (2)	140
C10—H10···O5^{ii}	0.95	2.56	3.4935 (18)	168

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