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[(*Z*)-2-(3-Methyl-1,2,4-oxadiazol-5-yl)-2-(1-naphthyl)ethenylamino]formaldehyde oxime 1,4-dioxane hemisolvate

Kensuke Okuda,[a] Hiromi Watanabe,[a] Takashi Hirota,[a] Kazuma Gotoh[b] and Hiroyuki Ishida[b]*

[a]Faculty of Pharmaceutical Sciences, Okayama University, Okayama 700-8530, Japan, and [b]Department of Chemistry, Faculty of Science, Okayama University, Okayama 700-8530, Japan
Correspondence e-mail: ishidah@cc.okayama-u.ac.jp

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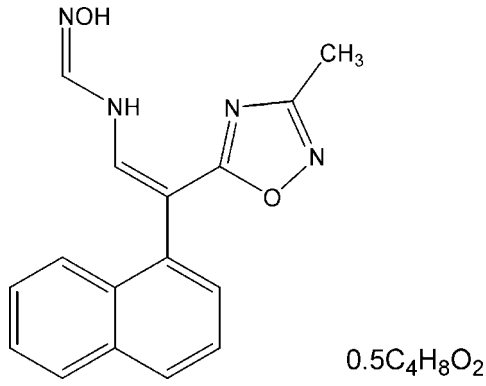
Key indicators: single-crystal X-ray study; T = 180 K; mean σ(C–C) = 0.002 Å; disorder in solvent or counterion; R factor = 0.047; wR factor = 0.137; data-to-parameter ratio = 20.1.

In the asymmetric unit of the title compound, $C_{16}H_{14}N_4O_2\cdot 0.5C_4H_8O_2$, there are two crystallographically independent oxime molecules and one solvent molecule. Each oxime molecule has intramolecular N—H···O and N—H···N hydrogen bonds, which make the non-H atoms approximately coplanar except for the naphthyl groups. The two independent molecules are connected to each other by O—H···N hydrogen bonds, forming a dimer. Dimers are linked into a layer through C—H···O, C—H···N and C—H···π interactions. There is π-stacking of approximately parallel oxadiazole rings, with a centroid–centroid distance of 3.6234 (9) Å and a dihedral angle of 8.90 (6)°. Dioxane C and H atoms are disordered over two sites each, with occupancy factors of *ca* 0.78:0.22.

Related literature

For related compounds, see: Okuda *et al.* (2007); Sasaki *et al.* (2001). For related literature, see: Frisch *et al.* (1998); Becke (1993); Lee *et al.* (1988).



Experimental

Crystal data

$C_{16}H_{14}N_4O_2\cdot 0.5C_4H_8O_2$
M_r = 338.37
Monoclinic, $C2/c$
a = 25.0090 (8) Å
b = 21.1940 (5) Å
c = 14.5843 (4) Å
β = 119.8098 (9)°
V = 6707.4 (3) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 180 (1) K
0.40 × 0.20 × 0.09 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: none
59998 measured reflections
9746 independent reflections
6472 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.137
S = 1.06
9746 reflections
486 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2*O*···N8	0.919 (19)	1.92 (2)	2.7733 (15)	153.4 (18)
O4—H4*O*···N4	0.93 (2)	1.91 (2)	2.7867 (15)	157 (2)
N3—H3*N*···O2	0.892 (16)	2.195 (15)	2.5413 (12)	102.4 (12)
N3—H3*N*···N2	0.892 (16)	2.081 (17)	2.7567 (15)	131.7 (13)
N7—H7*N*···O4	0.861 (16)	2.200 (15)	2.5337 (14)	102.8 (13)
N7—H7*N*···N6	0.861 (16)	2.136 (17)	2.7777 (16)	130.9 (13)
C4—H4···O4^{i}	0.93	2.50	3.0014 (16)	114
C15—H15···N1^{ii}	0.93	2.60	3.4675 (18)	155
C31—H31···N5^{iii}	0.93	2.45	3.3763 (17)	175
C33*A*—H33*A*···*Cg*1	0.97	2.87	3.501 (3)	123
C33*A*—H33*B*···*Cg*2^{iv}	0.97	2.93	3.804 (2)	150
C34*A*—H34*A*···*Cg*3^{iv}	0.97	2.93	3.575 (2)	125
C35*A*—H35*A*···*Cg*4^{i}	0.97	2.82	3.711 (2)	153
C33*B*—H33*C*···*Cg*2^{iv}	0.97	2.73	3.528 (9)	140
C35*B*—H35*D*···*Cg*4^{i}	0.97	2.69	3.408 (8)	131

Symmetry codes: (i) $x, -y, z+\frac{1}{2}$; (ii) $x, -y, z-\frac{1}{2}$; (iii) $x, -y+1, z+\frac{1}{2}$; (iv) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$. *Cg*1, *Cg*2, *Cg*3 and *Cg*4 are the centroids of the oxadiazole ring and the C21–C26, C17–C20/C25/C26 and C5–C10 benzene rings, respectively.

Data collection: *PROCESS-AUTO* (Rigaku/MSC, 2004); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure* and *PLATON* (Spek, 2003).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CF2149).

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supplementary materials

Acta Cryst. (2007). E**63**, o4261-o4262 [**doi:10.1107/S1600536807048301**]

[(*Z*)-2-(3-Methyl-1,2,4-oxadiazol-5-yl)-2-(1-naphthyl)ethenylamino]formaldehyde oxime 1,4-dioxane hemisolvate

K. Okuda, H. Watanabe, T. Hirota, K. Gotoh and H. Ishida

Comment

As part of our investigation to prepare anti-advanced glycation end-product (AGEs) agents, we have developed a pyrimidine ring-opening reaction accompanied by the formation of a 1,2,4-oxadiazole ring by the reaction of various 4-pyrimidinylamidines or their amide oximes with hydroxylamine hydrochloride (Sasaki *et al.*, 2001). The title compound, (I), was prepared for that purpose. A methanol solution of the compound on silica gel thin-layer chromatography (TLC) gave a single spot but it changed to two spots after one day, suggesting that the compound changed to an equilibrium mixture of two compounds. A methanol solution of the related compound, *N*-[5-(1-naphthyl)pyrimidin-4-yl]acetamide oxime, (II), which is a reaction substrate of the above reaction, has also shown a similar TLC phenomenon. Recently, we have determined the crystal structure of (II) by X-ray diffraction and interpreted this phenomenon in terms of two diastereomers of this compound caused by two sets of atropisomers which might exist in the methanol solution (Okuda *et al.*, 2007). In the present study, an X-ray crystal structure analysis of (I) was undertaken in order to obtain fundamental information about the TLC phenomenon.

In the asymmetric unit of (I), there are two crystallographically independent oxime molecules, A and B (Fig. 1). Each molecule has intramolecular N—H···O and N—H···N hydrogen bonds (Table 1), which make non-H atoms in the *N*-[(*Z*)-2-(3-methyl[1,2,4]oxadiazol-5-yl)-2-ethenyl]formamide oxime unit approximately coplanar; mean deviations from the defined plane are 0.0410 (12) and 0.0399 (12) Å for molecules A and B, respectively. Although bond lengths and angles of both molecules are essentially the same, the conformation of molecule A about the C1—C11 bond axis is quite different from that of B about C17—C27 as shown by torsion angles C2—C1—C11—C15 = 64.28 (17)° and C18—C17—C27—C31 = 122.24 (13)°. The dihedral angles between the naphthalene and the *N*-[(*Z*)-2-(3-methyl[1,2,4]oxadiazol-5-yl)-2-ethenyl]formamide oxime plane are 68.60 (2) and 57.88 (2)° for molecules A and B, respectively. Molecular orbital calculations at the HF/6–31 G** level of theory starting from geometries of A and B gave the same structure, the optimized torsion angle corresponding to C2—C1—C11—C15 or C18—C17—C27—C31 being 73.66°. The other stable structure was obtained as an atropisomer, the torsion angle being −73.66°.

In the crystal structure of (I), molecules A and B are connected to each other by O—H···N hydrogen bonds to form a dimer. Neighboring dimers related by a *c* glide plane are linked *via* C—H···O and C—H···N interactions, giving a molecular layer extending parallel to the (100) plane (Fig. 2). Adjacent layers are linked through a π-π stacking interaction between oxadiazole O1/N1/C13/N2/C12 rings which are approximately parallel to each other, forming a double layer structure (Fig. 3). The centroid-centroid [$Cg1\cdots Cg1^{v}$; symmetry code: (v) $1-x, y, 3/2-z$] distance of the oxadiazole rings is 3.6234 (9) Å and the dihedral angle between the rings is 8.90 (6)°; the shortest distance is $N2\cdots C13^{v}$ 3.398 (2) Å. The 1,4-dioxane molecules are placed in the void space between the molecular double layers (Fig. 3) and bound weakly through C—H···π interactions.

The oxime molecule of (I) gives only a set of atropisomers, which give the same spot on TLC. Therefore, for (I) we propose a different mechanism of the TLC phenomenon than we proposed for (II), based on the molecular structure. As shown in Fig. 4, in a methanol solution, equilibriation between compounds (Ia) and (Ib) is possible. We suggest the new spot on silica gel TLC is derived from (Ib). The compound, (Ib), is stable in the gas phase as confirmed by molecular orbital calculations at HF/6–31 G** and B3LYP/6–311 G** levels of theory, but the electric energy of (Ib) is much higher than that of (Ia). The differences between (Ia) and (Ib) calculated by B3LYP/6–311 G** and HF/6–31 G** are 56.64 and 70.49 kJ mol^{-1}, respectively, which might be reduced in a methanol solution but could govern the crystallized product. The oxime fragment of (Ib) is planar and intramolecular N—H···N and N—H···O hydrogen bonds are observed (N—H 1.041, H···N 1.806, N···N 2.581 Å and N—H···N 128.00°; N—H 1.041, H···O 2.755, N···O 3.774 Å and N—H···O 166.00° calculated by B3LYP/6–311 G**).

Experimental

To a methanol solution (15 ml) of *N*-[5-(1-naphthyl)pyrimidin-4-yl]acetamide oxime (139 mg, 0.5 mmol; Okuda *et al.*, 2007), hydroxylamine hydrochloride (46.3 mg, 0.6 mmol) was added. The mixture was stirred at room temperature for 3.5 h. After evaporation of methanol, 20 ml of water was added to the residue then it was extracted with ethyl acetate. The organic layer was washed with brine, dried over Na_2SO_4 and evaporated. The residue was recrystallized from methanol to give *N*-[(*Z*)-2-(3-methyl[1,2,4]oxadiazol-5-yl)-2-(1-naphthyl)ethenyl]formamide oxime (m.p. 483–486 K). Single crystals of (I) were obtained by recrystallization from a toluene:1,4-dioxane (2:1 *v*/*v*) solution (m.p. 464–465 K). After drying (I) at 393 K under vacuum, the melting temperature changed to 483–486 K.

Refinement

O-bound and N-bound H atoms were found in a difference Fourier map and refined isotropically (refined distances given in Table 1). Methyl H atoms were refined as riding, with C—H = 0.96 Å and with U_{iso}(H) = 1.5U_{eq}(C), allowing for rotation of the methyl group. Other H atoms were positioned geometrically (C—H = 0.93 or 0.97 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C). Atoms except for O in the dioxane molecule are disordered over two positions with site-occupation factors of 0.775 (4) and 0.225 (4). For the minor disorder component, distance restraints [O—C = 1.43 (1), C33B···C36B = 2.27 (2) and C34B···C35B = 2.27 (2) Å] were applied and the C atoms were refined isotropically.

The *ab initio* molecular calculations were performed by using the *GAUSSIAN98* package (Frisch *et al.*, 1998) at the HF/6–31 G** and B3LYP/6–311 G** (Becke, 1993; Lee *et al.*, 1988) levels of theory. Full optimizations were carried out and the resultant stable structures were confirmed by the vibrational analysis which shows only real frequencies for the optimized structures.

Figures

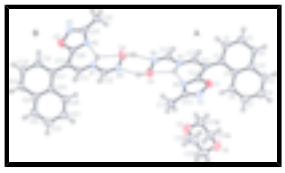


Fig. 1. The asymmetric unit of (I), showing two independent oxime molecules designated by A and B, and one disorder component of the dioxane molecule. Displacement ellipsoids for non-H atoms are drawn at the 40% probability level. Dashed lines indicate hydrogen bonds.

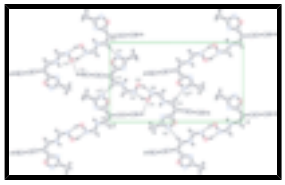


Fig. 2. A partial packing diagram of (I), viewed down the *a* axis, showing the molecular layer formed by hydrogen bonds (dashed lines). [Symmetry codes: (i) *x*,-*y*,1/2 + *z*; (ii) *x*,-*y*,-1/2 + *z*; (iii) *x*,1 − *y*,1/2 + *z*].

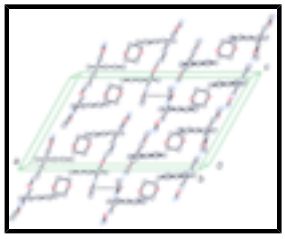


Fig. 3. A partial packing diagram of (I), viewed down the *b* axis, showing the molecular double layers formed by π-π interactions (dashed lines) and the dioxane molecules (major component) placed in the void space between the layers. H atoms have been omitted for clarity.

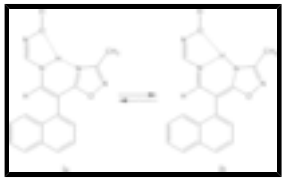


Fig. 4. Equilibrium between compounds (Ia) and (Ib)

[(*Z*)-2-(3-Methyl-1,2,4-oxadiazol-5-yl)-2-(1-naphthyl)ethenylamino]formaldehyde oxime 1,4-dioxane hemisolvate

Crystal data

$C_{16}H_{14}N_4O_2 \cdot 0.5C_4H_8O_2$	F_{000} = 2848.00
M_r = 338.37	D_x = 1.340 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71075 Å
Hall symbol: -C 2yc	Cell parameters from 37777 reflections
a = 25.0090 (8) Å	θ = 3.0–30.0º
b = 21.1940 (5) Å	μ = 0.09 mm^{-1}
c = 14.5843 (4) Å	*T* = 180 (1) K
β = 119.8098 (9)º	Plate, colorless
V = 6707.4 (3) Å^3	0.40 × 0.20 × 0.09 mm
Z = 16	

Data collection

Rigaku R-AXIS RAPID diffractometer	6472 reflections with $I > 2\sigma(I)$
Detector resolution: 10.00 pixels mm^{-1}	R_{int} = 0.049
T = 180(1) K	θ_{max} = 30.0º
ω scans	*h* = −35→35
Absorption correction: none	*k* = −29→29
59998 measured reflections	*l* = −20→18
9746 independent reflections	

Refinement

Refinement on F^2	6 restraints
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.047$	$w = 1/[\sigma^2(F_o^2) + (0.0753P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.137$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.06$	$\Delta\rho_{max} = 0.34$ e Å^{-3}
9746 reflections	$\Delta\rho_{min} = -0.26$ e Å^{-3}
486 parameters	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > 2$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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.42380 (4)	0.01354 (4)	0.75815 (6)	0.0352 (2)	
O2	0.41029 (5)	0.21271 (4)	0.46330 (7)	0.0392 (2)	
O3	0.41661 (5)	0.48641 (4)	−0.00821 (7)	0.0430 (3)	
O4	0.42264 (5)	0.28375 (4)	0.27960 (7)	0.0440 (3)	
O5	0.29391 (6)	0.16225 (6)	0.72011 (9)	0.0597 (3)	
O6	0.21126 (5)	0.08213 (5)	0.74108 (9)	0.0561 (3)	
N1	0.43588 (6)	0.06251 (5)	0.83317 (8)	0.0384 (3)	
N2	0.42091 (5)	0.10367 (5)	0.67926 (8)	0.0309 (2)	
N3	0.40594 (5)	0.09366 (4)	0.47936 (8)	0.0294 (2)	
N4	0.40493 (5)	0.17833 (5)	0.37562 (8)	0.0329 (2)	
N5	0.41912 (7)	0.43814 (5)	−0.07412 (9)	0.0464 (3)	
N6	0.41671 (5)	0.39517 (5)	0.06469 (8)	0.0297 (2)	
N7	0.42236 (5)	0.40251 (5)	0.25948 (8)	0.0307 (2)	
N8	0.42385 (5)	0.31816 (5)	0.36409 (8)	0.0343 (2)	
C1	0.40128 (6)	−0.06603 (5)	0.58731 (9)	0.0285 (2)	
C2	0.44715 (6)	−0.10320 (6)	0.59038 (10)	0.0354 (3)	
H2	0.4803	−0.0842	0.5890	0.042*	
C3	0.44503 (7)	−0.16939 (6)	0.59559 (11)	0.0399 (3)	
H3	0.4765	−0.1936	0.5970	0.048*	
C4	0.39731 (7)	−0.19811 (6)	0.59850 (10)	0.0374 (3)	

H4	0.3965	−0.2419	0.6022	0.045*
C5	0.29865 (7)	−0.19105 (6)	0.59899 (11)	0.0443 (3)
H5	0.2976	−0.2348	0.6036	0.053*
C6	0.25218 (8)	−0.15604 (8)	0.59526 (14)	0.0562 (4)
H6	0.2197	−0.1759	0.5977	0.067*
C7	0.25284 (7)	−0.08990 (8)	0.58778 (14)	0.0532 (4)
H7	0.2208	−0.0662	0.5851	0.064*
C8	0.30048 (6)	−0.06020 (6)	0.58438 (11)	0.0402 (3)
H8	0.3001	−0.0165	0.5785	0.048*
C9	0.35024 (6)	−0.09515 (5)	0.58971 (9)	0.0294 (2)
C10	0.34876 (6)	−0.16214 (5)	0.59594 (9)	0.0330 (3)
C11	0.40486 (6)	0.00385 (5)	0.58031 (9)	0.0282 (2)
C12	0.41573 (6)	0.04236 (5)	0.66965 (9)	0.0283 (2)
C13	0.43363 (6)	0.11357 (6)	0.78176 (9)	0.0324 (3)
C14	0.44440 (7)	0.17717 (6)	0.83035 (11)	0.0427 (3)
H14A	0.4790	0.1965	0.8298	0.064*
H14B	0.4528	0.1734	0.9019	0.064*
H14C	0.4084	0.2028	0.7908	0.064*
C15	0.40228 (6)	0.03038 (5)	0.49375 (9)	0.0294 (2)
H15	0.3977	0.0035	0.4399	0.035*
C16	0.40251 (6)	0.11929 (5)	0.39027 (9)	0.0304 (3)
H16	0.3981	0.0919	0.3371	0.036*
C17	0.40241 (6)	0.56352 (5)	0.13817 (9)	0.0278 (2)
C18	0.44426 (6)	0.60021 (6)	0.12689 (9)	0.0321 (3)
H18	0.4776	0.5810	0.1266	0.038*
C19	0.43748 (7)	0.66621 (6)	0.11577 (10)	0.0371 (3)
H19	0.4663	0.6900	0.1084	0.045*
C20	0.38901 (7)	0.69542 (6)	0.11579 (10)	0.0387 (3)
H20	0.3851	0.7390	0.1084	0.046*
C21	0.29388 (8)	0.68988 (7)	0.12774 (12)	0.0482 (4)
H21	0.2898	0.7335	0.1208	0.058*
C22	0.25137 (8)	0.65588 (8)	0.13840 (14)	0.0568 (4)
H22	0.2189	0.6762	0.1398	0.068*
C23	0.25652 (7)	0.58961 (8)	0.14730 (13)	0.0501 (4)
H23	0.2270	0.5665	0.1540	0.060*
C24	0.30426 (6)	0.55902 (6)	0.14627 (11)	0.0379 (3)
H24	0.3065	0.5153	0.1514	0.045*
C25	0.35057 (6)	0.59295 (5)	0.13752 (9)	0.0301 (2)
C26	0.34446 (6)	0.66003 (6)	0.12702 (10)	0.0353 (3)
C27	0.41140 (6)	0.49376 (5)	0.15171 (9)	0.0278 (2)
C28	0.41507 (6)	0.45665 (5)	0.07202 (9)	0.0280 (2)
C29	0.41883 (6)	0.38655 (6)	−0.02680 (9)	0.0318 (3)
C30	0.41975 (7)	0.32367 (6)	−0.07106 (11)	0.0400 (3)
H30A	0.3840	0.3001	−0.0834	0.060*
H30B	0.4562	0.3012	−0.0219	0.060*
H30C	0.4197	0.3290	−0.1365	0.060*
C31	0.41560 (6)	0.46548 (5)	0.23863 (9)	0.0293 (2)
H31	0.4137	0.4915	0.2883	0.035*
C32	0.42351 (6)	0.37709 (5)	0.34702 (9)	0.0311 (3)

H32	0.4241	0.4047	0.3971	0.037*	
C33A	0.27222 (11)	0.10533 (11)	0.66026 (16)	0.0487 (6)	0.775 (4)
H33A	0.3002	0.0710	0.6981	0.058*	0.775 (4)
H33B	0.2706	0.1104	0.5928	0.058*	0.775 (4)
C34A	0.21015 (11)	0.09049 (11)	0.64279 (15)	0.0478 (6)	0.775 (4)
H34A	0.1821	0.1245	0.6034	0.057*	0.775 (4)
H34B	0.1951	0.0522	0.6011	0.057*	0.775 (4)
C35A	0.23431 (12)	0.13985 (12)	0.80186 (17)	0.0511 (6)	0.775 (4)
H35A	0.2364	0.1349	0.8697	0.061*	0.775 (4)
H35B	0.2063	0.1743	0.7646	0.061*	0.775 (4)
C36A	0.29672 (11)	0.15494 (11)	0.81857 (16)	0.0534 (6)	0.775 (4)
H36A	0.3117	0.1936	0.8592	0.064*	0.775 (4)
H36B	0.3251	0.1212	0.8581	0.064*	0.775 (4)
C33B	0.2450 (5)	0.1294 (5)	0.6334 (7)	0.087 (4)*	0.225 (4)
H33C	0.2548	0.1221	0.5777	0.104*	0.225 (4)
H33D	0.2068	0.1530	0.6046	0.104*	0.225 (4)
C34B	0.2399 (6)	0.0672 (5)	0.6810 (10)	0.092 (4)*	0.225 (4)
H34C	0.2153	0.0372	0.6257	0.110*	0.225 (4)
H34D	0.2804	0.0492	0.7257	0.110*	0.225 (4)
C35B	0.2557 (5)	0.1152 (5)	0.8304 (6)	0.092 (4)*	0.225 (4)
H35C	0.2939	0.0916	0.8671	0.110*	0.225 (4)
H35D	0.2409	0.1242	0.8791	0.110*	0.225 (4)
C36B	0.2647 (6)	0.1766 (6)	0.7824 (9)	0.100 (4)*	0.225 (4)
H36C	0.2250	0.1964	0.7379	0.120*	0.225 (4)
H36D	0.2902	0.2058	0.8385	0.120*	0.225 (4)
H2O	0.4108 (8)	0.2538 (9)	0.4437 (14)	0.062 (5)*	
H4O	0.4161 (10)	0.2433 (10)	0.2957 (17)	0.085 (7)*	
H3N	0.4099 (7)	0.1200 (7)	0.5301 (13)	0.043 (4)*	
H7N	0.4220 (7)	0.3771 (7)	0.2131 (13)	0.043 (4)*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0532 (6)	0.0262 (4)	0.0302 (4)	−0.0033 (4)	0.0238 (4)	0.0004 (3)
O2	0.0666 (7)	0.0240 (4)	0.0340 (5)	−0.0025 (4)	0.0304 (5)	−0.0008 (4)
O3	0.0778 (8)	0.0276 (4)	0.0354 (5)	0.0014 (4)	0.0371 (5)	0.0029 (4)
O4	0.0800 (8)	0.0252 (4)	0.0388 (5)	0.0017 (4)	0.0387 (5)	0.0006 (4)
O5	0.0633 (8)	0.0560 (7)	0.0584 (7)	−0.0165 (6)	0.0292 (6)	0.0007 (5)
O6	0.0558 (7)	0.0542 (6)	0.0612 (7)	−0.0083 (5)	0.0312 (6)	0.0046 (5)
N1	0.0556 (7)	0.0328 (6)	0.0307 (5)	−0.0035 (5)	0.0244 (5)	−0.0038 (4)
N2	0.0426 (6)	0.0246 (5)	0.0293 (5)	−0.0032 (4)	0.0209 (5)	−0.0018 (4)
N3	0.0429 (6)	0.0220 (5)	0.0283 (5)	−0.0025 (4)	0.0215 (5)	−0.0004 (4)
N4	0.0472 (7)	0.0272 (5)	0.0288 (5)	−0.0010 (4)	0.0223 (5)	−0.0003 (4)
N5	0.0814 (10)	0.0322 (6)	0.0383 (6)	0.0018 (6)	0.0394 (7)	−0.0007 (5)
N6	0.0383 (6)	0.0255 (5)	0.0296 (5)	0.0017 (4)	0.0201 (4)	0.0011 (4)
N7	0.0453 (6)	0.0241 (5)	0.0271 (5)	0.0028 (4)	0.0213 (5)	0.0014 (4)
N8	0.0500 (7)	0.0287 (5)	0.0278 (5)	0.0011 (4)	0.0220 (5)	0.0007 (4)
C1	0.0382 (7)	0.0221 (5)	0.0268 (5)	−0.0008 (4)	0.0174 (5)	0.0007 (4)

C2	0.0426 (8)	0.0288 (6)	0.0405 (7)	0.0003 (5)	0.0250 (6)	0.0017 (5)
C3	0.0520 (9)	0.0287 (6)	0.0435 (7)	0.0093 (6)	0.0271 (7)	0.0036 (5)
C4	0.0588 (9)	0.0210 (5)	0.0323 (6)	0.0018 (5)	0.0226 (6)	0.0033 (5)
C5	0.0517 (9)	0.0337 (7)	0.0446 (8)	−0.0138 (6)	0.0218 (7)	0.0010 (6)
C6	0.0486 (10)	0.0535 (9)	0.0716 (11)	−0.0178 (7)	0.0336 (9)	−0.0003 (8)
C7	0.0414 (9)	0.0512 (9)	0.0729 (11)	−0.0033 (7)	0.0329 (8)	−0.0022 (8)
C8	0.0396 (8)	0.0327 (6)	0.0483 (8)	−0.0029 (5)	0.0218 (6)	−0.0019 (6)
C9	0.0361 (7)	0.0248 (5)	0.0269 (5)	−0.0028 (5)	0.0154 (5)	−0.0007 (4)
C10	0.0457 (8)	0.0249 (5)	0.0269 (5)	−0.0058 (5)	0.0170 (5)	−0.0003 (4)
C11	0.0358 (7)	0.0204 (5)	0.0316 (6)	−0.0016 (4)	0.0192 (5)	−0.0004 (4)
C12	0.0340 (6)	0.0250 (5)	0.0291 (6)	−0.0012 (4)	0.0182 (5)	0.0018 (4)
C13	0.0405 (7)	0.0303 (6)	0.0296 (6)	−0.0032 (5)	0.0197 (5)	−0.0017 (5)
C14	0.0615 (10)	0.0321 (7)	0.0373 (7)	−0.0055 (6)	0.0267 (7)	−0.0092 (5)
C15	0.0374 (7)	0.0229 (5)	0.0316 (6)	−0.0016 (4)	0.0201 (5)	−0.0019 (4)
C16	0.0418 (7)	0.0264 (6)	0.0280 (5)	−0.0011 (5)	0.0212 (5)	−0.0011 (4)
C17	0.0357 (6)	0.0243 (5)	0.0222 (5)	−0.0006 (4)	0.0135 (5)	0.0006 (4)
C18	0.0381 (7)	0.0293 (6)	0.0291 (6)	−0.0013 (5)	0.0169 (5)	0.0022 (5)
C19	0.0476 (8)	0.0307 (6)	0.0338 (6)	−0.0081 (5)	0.0208 (6)	0.0012 (5)
C20	0.0571 (9)	0.0226 (5)	0.0357 (6)	−0.0022 (5)	0.0224 (6)	0.0006 (5)
C21	0.0575 (10)	0.0351 (7)	0.0526 (8)	0.0121 (6)	0.0279 (8)	0.0011 (6)
C22	0.0501 (10)	0.0554 (10)	0.0716 (11)	0.0152 (7)	0.0355 (9)	0.0022 (8)
C23	0.0414 (9)	0.0533 (9)	0.0616 (9)	0.0025 (7)	0.0302 (8)	0.0038 (7)
C24	0.0383 (7)	0.0335 (6)	0.0424 (7)	0.0000 (5)	0.0205 (6)	0.0025 (5)
C25	0.0357 (7)	0.0276 (6)	0.0252 (5)	0.0013 (5)	0.0138 (5)	0.0008 (4)
C26	0.0460 (8)	0.0278 (6)	0.0308 (6)	0.0032 (5)	0.0181 (6)	0.0002 (5)
C27	0.0342 (6)	0.0236 (5)	0.0268 (5)	0.0012 (4)	0.0161 (5)	0.0009 (4)
C28	0.0320 (6)	0.0275 (5)	0.0253 (5)	0.0013 (4)	0.0149 (5)	0.0050 (4)
C29	0.0368 (7)	0.0315 (6)	0.0300 (6)	0.0004 (5)	0.0187 (5)	0.0005 (5)
C30	0.0525 (9)	0.0335 (6)	0.0408 (7)	−0.0007 (6)	0.0283 (7)	−0.0061 (6)
C31	0.0369 (7)	0.0239 (5)	0.0285 (6)	0.0008 (4)	0.0174 (5)	0.0003 (4)
C32	0.0429 (7)	0.0269 (6)	0.0255 (5)	0.0012 (5)	0.0186 (5)	0.0026 (4)
C33A	0.0513 (13)	0.0569 (12)	0.0387 (10)	−0.0011 (10)	0.0232 (9)	−0.0082 (9)
C34A	0.0467 (12)	0.0533 (12)	0.0371 (10)	−0.0093 (9)	0.0161 (9)	−0.0142 (9)
C35A	0.0533 (13)	0.0668 (14)	0.0339 (9)	0.0019 (11)	0.0221 (9)	−0.0081 (10)
C36A	0.0543 (14)	0.0576 (13)	0.0370 (10)	−0.0090 (10)	0.0141 (10)	−0.0139 (9)

Geometric parameters (Å, °)

O1—C12	1.3493 (13)	C14—H14A	0.96
O1—N1	1.4272 (13)	C14—H14B	0.96
O2—N4	1.4191 (13)	C14—H14C	0.96
O2—H2O	0.918 (19)	C15—H15	0.93
O3—C28	1.3467 (13)	C16—H16	0.93
O3—N5	1.4263 (13)	C17—C18	1.3777 (16)
O4—N8	1.4192 (13)	C17—C25	1.4346 (17)
O4—H4O	0.92 (2)	C17—C27	1.4937 (15)
O5—C36A	1.411 (2)	C18—C19	1.4087 (17)
O5—C33B	1.430 (7)	C18—H18	0.93
O5—C33A	1.429 (2)	C19—C20	1.361 (2)

O5—C36B	1.453 (5)	C19—H19	0.93
O6—C34B	1.417 (5)	C20—C26	1.4184 (19)
O6—C35B	1.409 (5)	C20—H20	0.93
O6—C34A	1.431 (2)	C21—C22	1.356 (2)
O6—C35A	1.451 (2)	C21—C26	1.419 (2)
N1—C13	1.3017 (16)	C21—H21	0.93
N2—C12	1.3066 (14)	C22—C23	1.411 (2)
N2—C13	1.3809 (15)	C22—H22	0.93
N3—C15	1.3674 (14)	C23—C24	1.3652 (19)
N3—C16	1.3711 (14)	C23—H23	0.93
N3—H3N	0.892 (15)	C24—C25	1.4218 (17)
N4—C16	1.2757 (14)	C24—H24	0.93
N5—C29	1.2949 (16)	C25—C26	1.4299 (16)
N6—C28	1.3098 (14)	C27—C31	1.3583 (15)
N6—C29	1.3738 (15)	C27—C28	1.4435 (15)
N7—C31	1.3606 (14)	C29—C30	1.4859 (17)
N7—C32	1.3727 (14)	C30—H30A	0.96
N7—H7N	0.861 (15)	C30—H30B	0.96
N8—C32	1.2727 (14)	C30—H30C	0.96
C1—C2	1.3738 (17)	C31—H31	0.93
C1—C9	1.4337 (16)	C32—H32	0.93
C1—C11	1.4904 (15)	C33A—C34A	1.477 (3)
C2—C3	1.4073 (17)	C33A—H33A	0.97
C2—H2	0.93	C33A—H33B	0.97
C3—C4	1.359 (2)	C34A—H34A	0.97
C3—H3	0.93	C34A—H34B	0.97
C4—C10	1.4184 (19)	C35A—C36A	1.490 (3)
C4—H4	0.93	C35A—H35A	0.97
C5—C6	1.357 (2)	C35A—H35B	0.97
C5—C10	1.4155 (19)	C36A—H36A	0.97
C5—H5	0.93	C36A—H36B	0.97
C6—C7	1.407 (2)	C33B—C34B	1.523 (13)
C6—H6	0.93	C33B—H33C	0.97
C7—C8	1.370 (2)	C33B—H33D	0.97
C7—H7	0.93	C34B—H34C	0.97
C8—C9	1.4169 (18)	C34B—H34D	0.97
C8—H8	0.93	C35B—C36B	1.545 (14)
C9—C10	1.4244 (16)	C35B—H35C	0.97
C11—C15	1.3540 (16)	C35B—H35D	0.97
C11—C12	1.4440 (16)	C36B—H36C	0.97
C13—C14	1.4839 (16)	C36B—H36D	0.97
C12—O1—N1	106.15 (8)	C26—C21—H21	119.5
N4—O2—H2O	102.5 (11)	C21—C22—C23	119.92 (14)
C28—O3—N5	106.23 (9)	C21—C22—H22	120.0
N8—O4—H4O	100.8 (13)	C23—C22—H22	120.0
C33A—O5—C36A	109.92 (14)	C24—C23—C22	120.81 (14)
C34A—O6—C35A	108.15 (14)	C24—C23—H23	119.6
C33B—O5—C36B	100.4 (6)	C22—C23—H23	119.6
C34B—O6—C35B	105.8 (7)	C23—C24—C25	121.11 (13)

C13—N1—O1	103.35 (9)	C23—C24—H24	119.4
C12—N2—C13	102.96 (9)	C25—C24—H24	119.4
C15—N3—C16	123.82 (10)	C24—C25—C26	117.64 (11)
C15—N3—H3N	118.3 (9)	C24—C25—C17	123.59 (11)
C16—N3—H3N	117.9 (9)	C26—C25—C17	118.76 (11)
C16—N4—O2	110.11 (9)	C20—C26—C21	121.28 (12)
C29—N5—O3	103.46 (9)	C20—C26—C25	119.33 (12)
C28—N6—C29	103.27 (9)	C21—C26—C25	119.39 (12)
C31—N7—C32	122.39 (10)	C31—C27—C28	120.30 (10)
C31—N7—H7N	119.0 (10)	C31—C27—C17	119.80 (10)
C32—N7—H7N	118.3 (10)	C28—C27—C17	119.90 (9)
C32—N8—O4	109.83 (9)	N6—C28—O3	112.30 (10)
C2—C1—C9	119.44 (11)	N6—C28—C27	128.68 (10)
C2—C1—C11	119.63 (11)	O3—C28—C27	119.03 (10)
C9—C1—C11	120.93 (10)	N5—C29—N6	114.74 (11)
C1—C2—C3	121.33 (12)	N5—C29—C30	121.36 (11)
C1—C2—H2	119.3	N6—C29—C30	123.90 (11)
C3—C2—H2	119.3	C29—C30—H30A	109.5
C4—C3—C2	120.37 (12)	C29—C30—H30B	109.5
C4—C3—H3	119.8	H30A—C30—H30B	109.5
C2—C3—H3	119.8	C29—C30—H30C	109.5
C3—C4—C10	120.79 (11)	H30A—C30—H30C	109.5
C3—C4—H4	119.6	H30B—C30—H30C	109.5
C10—C4—H4	119.6	C27—C31—N7	125.79 (10)
C6—C5—C10	121.06 (13)	C27—C31—H31	117.1
C6—C5—H5	119.5	N7—C31—H31	117.1
C10—C5—H5	119.5	N8—C32—N7	124.21 (11)
C5—C6—C7	120.35 (14)	N8—C32—H32	117.9
C5—C6—H6	119.8	N7—C32—H32	117.9
C7—C6—H6	119.8	O5—C33A—C34A	109.42 (17)
C8—C7—C6	120.30 (15)	O5—C33A—H33A	109.8
C8—C7—H7	119.8	C34A—C33A—H33A	109.8
C6—C7—H7	119.8	O5—C33A—H33B	109.8
C7—C8—C9	120.92 (13)	C34A—C33A—H33B	109.8
C7—C8—H8	119.5	H33A—C33A—H33B	108.2
C9—C8—H8	119.5	O6—C34A—C33A	111.00 (16)
C8—C9—C10	118.32 (11)	O6—C34A—H34A	109.4
C8—C9—C1	122.82 (11)	C33A—C34A—H34A	109.4
C10—C9—C1	118.84 (11)	O6—C34A—H34B	109.4
C5—C10—C4	121.75 (11)	C33A—C34A—H34B	109.4
C5—C10—C9	119.02 (12)	H34A—C34A—H34B	108.0
C4—C10—C9	119.23 (11)	O6—C35A—C36A	110.28 (17)
C15—C11—C12	120.46 (10)	O6—C35A—H35A	109.6
C15—C11—C1	119.99 (10)	C36A—C35A—H35A	109.6
C12—C11—C1	119.38 (10)	O6—C35A—H35B	109.6
N2—C12—O1	112.82 (10)	C36A—C35A—H35B	109.6
N2—C12—C11	128.54 (10)	H35A—C35A—H35B	108.1
O1—C12—C11	118.61 (10)	O5—C36A—C35A	109.82 (17)
N1—C13—N2	114.71 (11)	O5—C36A—H36A	109.7

N1—C13—C14	122.31 (11)	C35A—C36A—H36A	109.7
N2—C13—C14	122.98 (11)	O5—C36A—H36B	109.7
C13—C14—H14A	109.5	C35A—C36A—H36B	109.7
C13—C14—H14B	109.5	H36A—C36A—H36B	108.2
H14A—C14—H14B	109.5	O5—C33B—C34B	104.3 (8)
C13—C14—H14C	109.5	O5—C33B—H33C	110.9
H14A—C14—H14C	109.5	C34B—C33B—H33C	110.9
H14B—C14—H14C	109.5	O5—C33B—H33D	110.9
C11—C15—N3	125.07 (10)	C34B—C33B—H33D	110.9
C11—C15—H15	117.5	H33C—C33B—H33D	108.9
N3—C15—H15	117.5	O6—C34B—C33B	105.8 (8)
N4—C16—N3	124.16 (10)	O6—C34B—H34C	110.6
N4—C16—H16	117.9	C33B—C34B—H34C	110.6
N3—C16—H16	117.9	O6—C34B—H34D	110.6
C18—C17—C25	119.43 (11)	C33B—C34B—H34D	110.6
C18—C17—C27	120.08 (11)	H34C—C34B—H34D	108.7
C25—C17—C27	120.49 (10)	O6—C35B—C36B	103.1 (8)
C17—C18—C19	121.28 (12)	O6—C35B—H35C	111.1
C17—C18—H18	119.4	C36B—C35B—H35C	111.1
C19—C18—H18	119.4	O6—C35B—H35D	111.1
C20—C19—C18	120.51 (12)	C36B—C35B—H35D	111.1
C20—C19—H19	119.7	H35C—C35B—H35D	109.1
C18—C19—H19	119.7	O5—C36B—C35B	109.7 (8)
C19—C20—C26	120.68 (11)	O5—C36B—H36C	109.7
C19—C20—H20	119.7	C35B—C36B—H36C	109.7
C26—C20—H20	119.7	O5—C36B—H36D	109.7
C22—C21—C26	121.10 (13)	C35B—C36B—H36D	109.7
C22—C21—H21	119.5	H36C—C36B—H36D	108.2
C12—O1—N1—C13	0.02 (13)	C21—C22—C23—C24	0.6 (3)
C28—O3—N5—C29	−0.04 (15)	C22—C23—C24—C25	0.8 (2)
C9—C1—C2—C3	0.15 (18)	C23—C24—C25—C26	−1.63 (19)
C11—C1—C2—C3	−179.16 (11)	C23—C24—C25—C17	178.69 (13)
C1—C2—C3—C4	−0.5 (2)	C18—C17—C25—C24	178.56 (11)
C2—C3—C4—C10	0.25 (19)	C27—C17—C25—C24	−1.87 (17)
C10—C5—C6—C7	0.3 (2)	C18—C17—C25—C26	−1.12 (16)
C5—C6—C7—C8	−0.1 (3)	C27—C17—C25—C26	178.45 (10)
C6—C7—C8—C9	−0.9 (2)	C19—C20—C26—C21	179.66 (13)
C7—C8—C9—C10	1.61 (19)	C19—C20—C26—C25	−0.51 (19)
C7—C8—C9—C1	−179.46 (13)	C22—C21—C26—C20	179.94 (14)
C2—C1—C9—C8	−178.51 (12)	C22—C21—C26—C25	0.1 (2)
C11—C1—C9—C8	0.79 (17)	C24—C25—C26—C20	−178.65 (11)
C2—C1—C9—C10	0.41 (17)	C17—C25—C26—C20	1.05 (17)
C11—C1—C9—C10	179.71 (10)	C24—C25—C26—C21	1.18 (18)
C6—C5—C10—C4	−179.23 (14)	C17—C25—C26—C21	−179.12 (11)
C6—C5—C10—C9	0.5 (2)	C18—C17—C27—C31	122.24 (13)
C3—C4—C10—C5	−179.94 (12)	C25—C17—C27—C31	−57.32 (16)
C3—C4—C10—C9	0.32 (18)	C18—C17—C27—C28	−58.27 (16)
C8—C9—C10—C5	−1.42 (17)	C25—C17—C27—C28	122.16 (12)
C1—C9—C10—C5	179.60 (11)	C29—N6—C28—O3	−0.57 (14)

C8—C9—C10—C4	178.33 (11)	C29—N6—C28—C27	178.81 (13)
C1—C9—C10—C4	−0.64 (17)	N5—O3—C28—N6	0.40 (14)
C2—C1—C11—C15	64.28 (17)	N5—O3—C28—C27	−179.04 (11)
C9—C1—C11—C15	−115.02 (13)	C31—C27—C28—N6	6.9 (2)
C2—C1—C11—C12	−111.09 (13)	C17—C27—C28—N6	−172.63 (12)
C9—C1—C11—C12	69.62 (15)	C31—C27—C28—O3	−173.80 (11)
C13—N2—C12—O1	0.48 (14)	C17—C27—C28—O3	6.72 (17)
C13—N2—C12—C11	−177.37 (13)	O3—N5—C29—N6	−0.33 (16)
N1—O1—C12—N2	−0.33 (14)	O3—N5—C29—C30	178.75 (12)
N1—O1—C12—C11	177.76 (11)	C28—N6—C29—N5	0.57 (16)
C15—C11—C12—N2	4.0 (2)	C28—N6—C29—C30	−178.49 (13)
C1—C11—C12—N2	179.29 (12)	C28—C27—C31—N7	−1.07 (19)
C15—C11—C12—O1	−173.79 (11)	C17—C27—C31—N7	178.42 (11)
C1—C11—C12—O1	1.55 (17)	C32—N7—C31—C27	−177.01 (12)
O1—N1—C13—N2	0.29 (15)	O4—N8—C32—N7	−0.20 (18)
O1—N1—C13—C14	−179.27 (12)	C31—N7—C32—N8	173.02 (12)
C12—N2—C13—N1	−0.48 (15)	C36A—O5—C33A—C34A	59.9 (2)
C12—N2—C13—C14	179.08 (13)	C35A—O6—C34A—C33A	58.7 (2)
C12—C11—C15—N3	−3.8 (2)	O5—C33A—C34A—O6	−60.1 (2)
C1—C11—C15—N3	−179.08 (11)	C34A—O6—C35A—C36A	−57.9 (2)
C16—N3—C15—C11	−179.25 (12)	C33A—O5—C36A—C35A	−59.8 (3)
O2—N4—C16—N3	−1.23 (17)	O6—C35A—C36A—O5	59.3 (3)
C15—N3—C16—N4	178.86 (12)	C36B—O5—C33B—C34B	−69.8 (9)
C25—C17—C18—C19	0.65 (17)	C35B—O6—C34B—C33B	−71.7 (11)
C27—C17—C18—C19	−178.92 (11)	O5—C33B—C34B—O6	74.5 (11)
C17—C18—C19—C20	−0.10 (18)	C34B—O6—C35B—C36B	65.7 (11)
C18—C19—C20—C26	0.02 (19)	C33B—O5—C36B—C35B	69.5 (10)
C26—C21—C22—C23	−1.0 (2)	O6—C35B—C36B—O5	−67.7 (12)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2O···N8	0.919 (19)	1.92 (2)	2.7733 (15)	153.4 (18)
O4—H4O···N4	0.93 (2)	1.91 (2)	2.7867 (15)	157 (2)
N3—H3N···O2	0.892 (16)	2.195 (15)	2.5413 (12)	102.4 (12)
N3—H3N···N2	0.892 (16)	2.081 (17)	2.7567 (15)	131.7 (13)
N7—H7N···O4	0.861 (16)	2.200 (15)	2.5337 (14)	102.8 (13)
N7—H7N···N6	0.861 (16)	2.136 (17)	2.7777 (16)	130.9 (13)
C4—H4···O4^{i}	0.93	2.50	3.0014 (16)	114
C15—H15···N1^{ii}	0.93	2.60	3.4675 (18)	155
C31—H31···N5^{iii}	0.93	2.45	3.3763 (17)	175
C33A—H33A···Cg1	0.97	2.87	3.501 (3)	123
C33A—H33B···Cg2^{iv}	0.97	2.93	3.804 (2)	150
C34A—H34A···Cg3^{iv}	0.97	2.93	3.575 (2)	125
C35A—H35A···Cg4^{i}	0.97	2.82	3.711 (2)	153
C33B—H33C···Cg2^{iv}	0.97	2.73	3.528 (9)	140
C35B—H35D···Cg4^{i}	0.97	2.69	3.408 (8)	131

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

Fig. 1

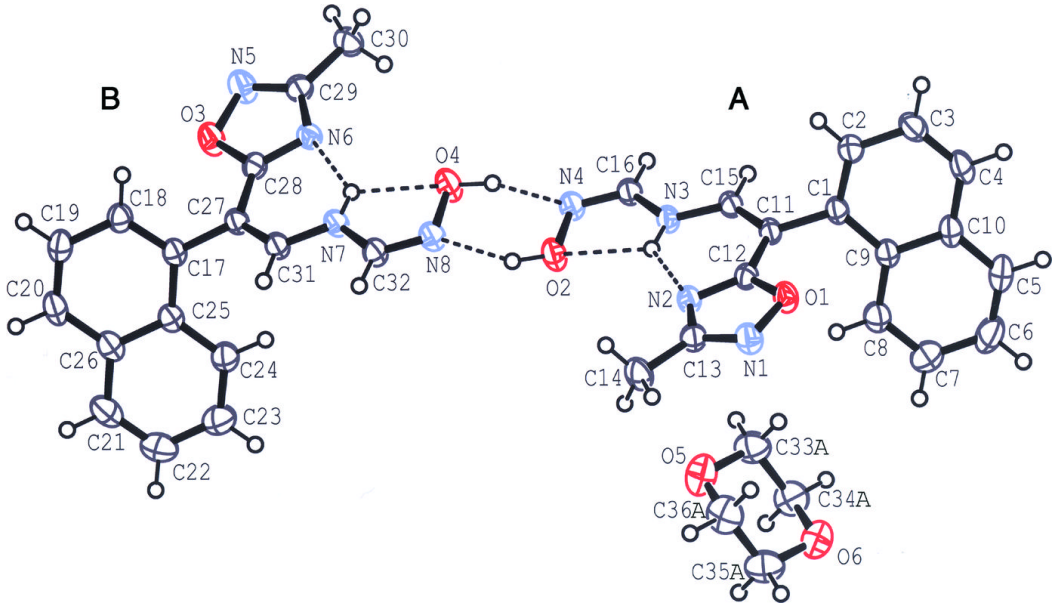


Fig. 2

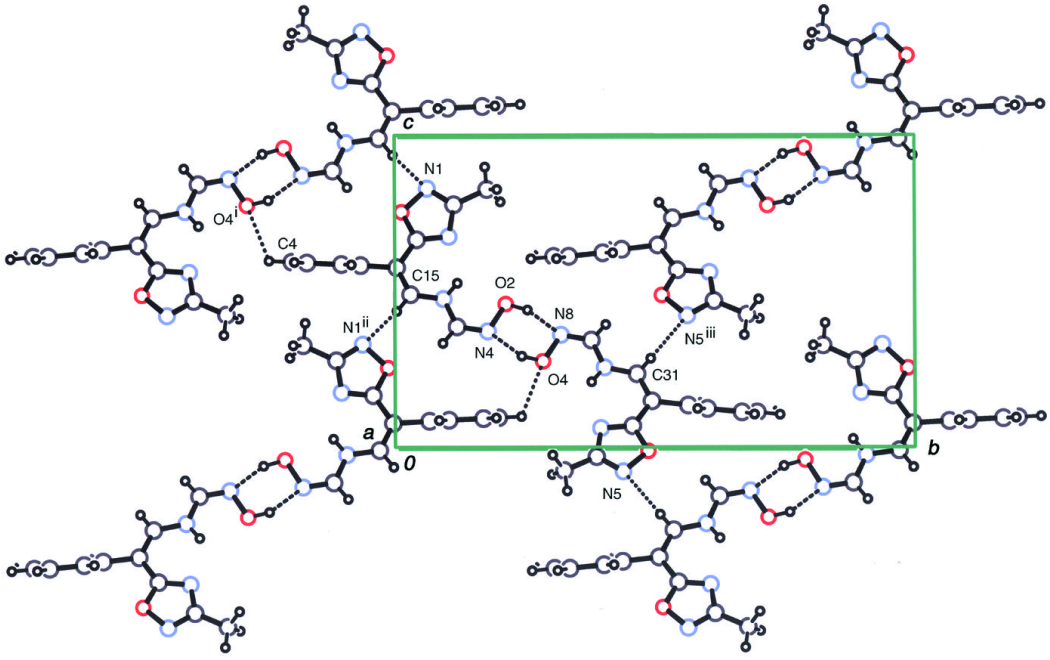


Fig. 3

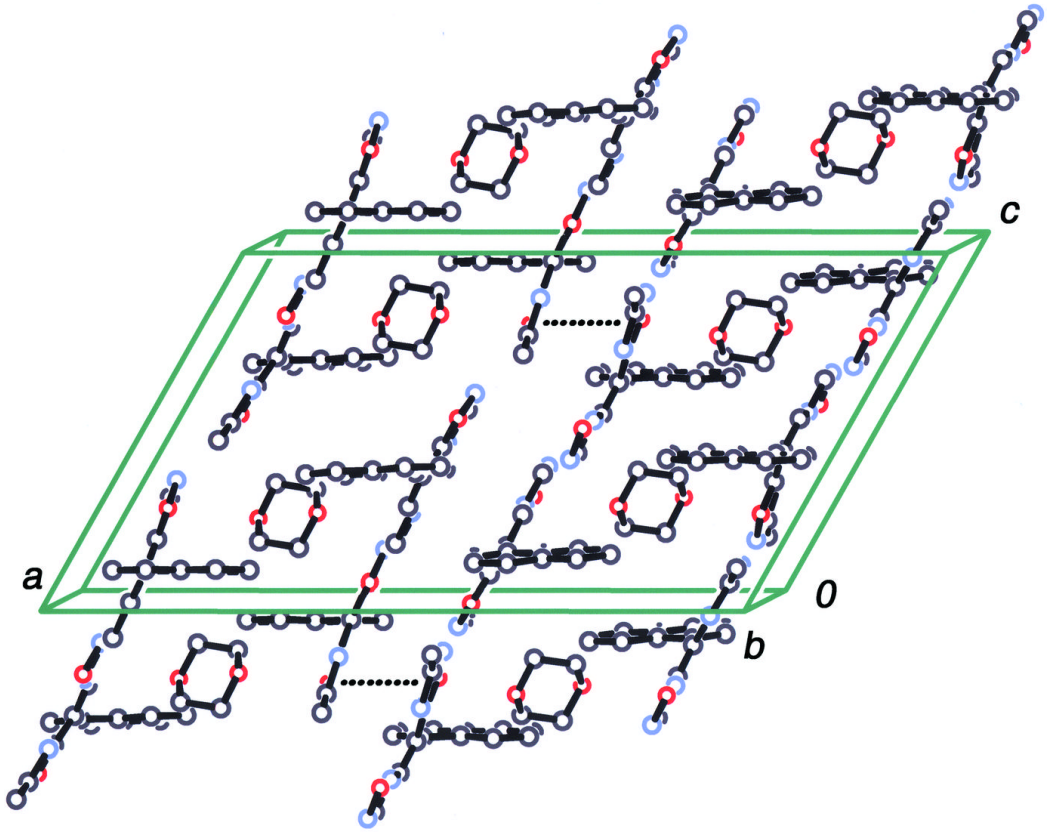
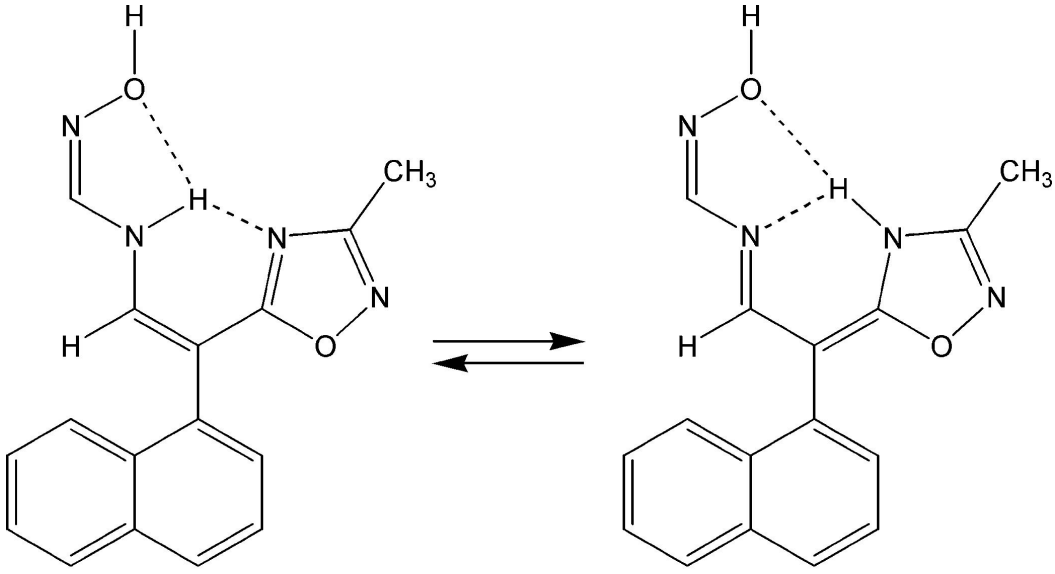


Fig. 4



Ia Ib