Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Hydrogen-bonded chains in 1-[3-(4-nitrobenzylideneamino)propyl]-2-(4-nitrophenyl)-hexahydropyrimidine methanol solvate

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.004 Å
R factor = 0.083
wR factor = 0.222
Data-to-parameter ratio = 16.7

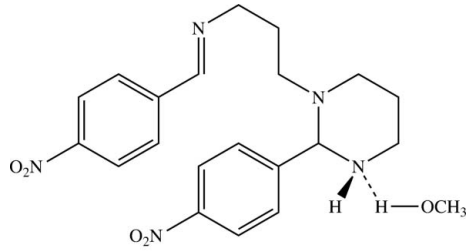
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 7 August 2006
Accepted 8 August 2006

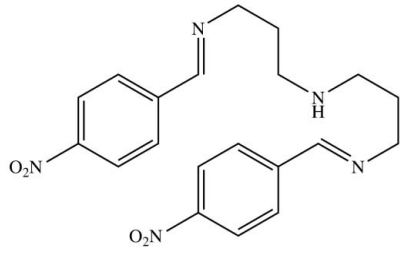
In the title compound, $C_{20}H_{23}N_5O_4\cdot CH_4O$, the molecular components are linked into $C_2^2(4)$ chains by a combination of O—H···N and N—H···O hydrogen bonds.

Comment

We report here the structure of the title compound, (I) (Fig. 1), a stoichiometric methanol solvate, wherein the pyrimidine component was formed by spontaneous cyclization of the intermediate (II) (see scheme) produced by condensation of bis(3-aminopropyl)amine with two molar equivalents of 4-nitrobenzaldehyde. We have recently reported the supramolecular structures of the 4-nitrobenzylidene derivatives of 1,2-diaminoethane and 1,3-diaminopropane (Bomfim *et al.*, 2005), 1,8-diaminooctane (Glidewell *et al.*, 2005*b*) and tris(2-aminoethyl)amine (Glidewell *et al.*, 2005*a*). The target compound, (II), was intended to complement that series but, in the event, the ring-closed product (I) resulted.



(I)



(II)

For the hexahydropyrimidine ring (N11/C12/N13/C14–C16), the ring-puckering parameters [θ = 176.1 (3)° and φ = 162 (5)°; Cremer & Pople, 1975] indicate an almost perfect chair conformation. The substituents at N11 and C12 both occupy equatorial sites, as expected, but the N—H bond at N13 occupies an axial site with the lone pair at N13 equatorial. The bond lengths and angles show no unexpected features.

Within the selected asymmetric unit (Fig. 1) the components are linked by an almost linear O—H···N hydrogen bond (Table 1). In addition, atom N13 at (*x*, *y*, *z*) acts as hydrogen-

bond donor to methanol atom O41 at $(1-x, \frac{1}{2}+y, \frac{3}{2}-z)$, so forming a $C_2^2(4)$ (Bernstein *et al.*, 1995) chain running parallel to the [010] direction and generated by the 2_1 screw axis along $(\frac{1}{2}, y, \frac{3}{4})$ (Fig. 2). Two such chains, related to one another by inversion and hence antiparallel, pass through each unit cell, but there are no significant direction-specific interactions between adjacent chains. Two C—H···O contacts between chains (Table 1) both involve aliphatic C—H bonds of very low acidity, both are long, and hence are probably not structurally significant.

Experimental

A solution of 4-nitrobenazaldehyde (4 mmol) and bis(3-aminopropyl)amine (2 mmol) in methanol (25 ml) was heated under reflux for 2 h. The mixture was cooled to ambient temperature and the solvent was removed under reduced pressure. Recrystallization of the crude solid product from methanol provided crystals of compound (I) suitable for single-crystal X-ray diffraction.

Crystal data

$C_{20}H_{23}N_5O_4\cdot CH_4O$
$M_r = 429.48$
Monoclinic, $P2_1/c$
$a = 16.9257\ (16)$ Å
$b = 7.5144\ (8)$ Å
$c = 16.8911\ (15)$ Å
$\beta = 93.562\ (5)^\circ$
$V = 2144.2\ (4)$ Å^3
$Z = 4$
$D_x = 1.330$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.10$ mm^{-1}
$T = 120\ (2)$ K
Plate, colourless
0.24 × 0.22 × 0.06 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min} = 0.965$, $T_{max} = 0.994$
23793 measured reflections
4712 independent reflections
3010 reflections with $I > 2\sigma(I)$
$R_{int} = 0.067$
$\theta_{max} = 27.5^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.083$
$wR(F^2) = 0.222$
$S = 1.08$
4712 reflections
282 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0907P)^2 + 2.3771P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}

Table 1
Hydrogen bonds and short intermolecular contacts (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O41—H41···N13	0.84	1.94	2.782 (4)	178
N13—H13···O41^{i}	0.88	1.97	2.841 (3)	171
C17—H17B···O32^{ii}	0.99	2.55	3.371 (4)	140
C18—H18A···O31^{iii}	0.99	2.56	3.490 (4)	156

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (iii) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

All H atoms were located in difference maps and then treated as riding atoms, with C—H = 0.95 (aromatic and =CH—), 0.98 (CH_3), 0.99 (CH_2) or 1.00 Å (aliphatic CH), N—H = 0.88 Å and O—H = 0.84 Å, and with $U_{iso}(H) = kU_{eq}(C,N,O)$, where $k = 1.5$ for the methanol H atoms and 1.2 for all other H atoms.

Data collection: *COLLECT* (Hooft, 1999); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *OSCAIL* (McArdle, 2003) and *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PRPKAPPA* (Ferguson, 1999).

X-ray data were collected at the EPSRC National X-ray Crystallography Service, University of Southampton, England, using a Nonius KappaCCD diffractometer. The

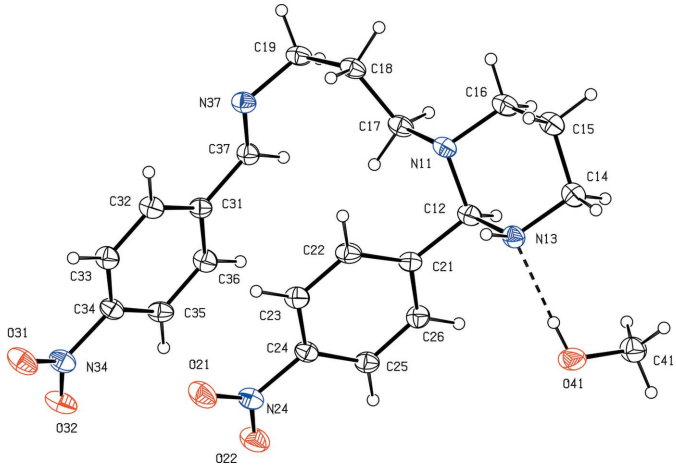


Figure 1
The molecular components of compound (I), showing the atom-labelling scheme and the O—H···N hydrogen bond (dashed line) within the selected asymmetric unit. Displacement ellipsoids are drawn at the 30% probability level.

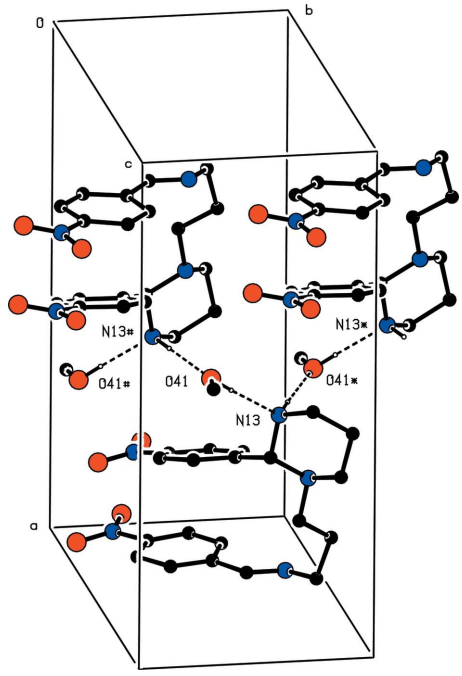


Figure 2
Part of the crystal structure of compound (I), showing the formation of a $C_2^2(4)$ chain along [010]. For the sake of clarity, H atoms not involved in the motif shown have been omitted. Atoms marked with an asterisk (*) or a hash (#) are at the symmetry positions $(1-x, \frac{1}{2}+y, \frac{3}{2}-z)$ and $(1-x, -\frac{1}{2}+y, \frac{3}{2}-z)$, respectively. Dashed lines indicate hydrogen bonds.

authors thank the staff for all their help and advice. JLW thanks CNPq and FAPERJ for financial support.

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supporting information

Acta Cryst. (2006). E**62**, o3844–o3846 [https://doi.org/10.1107/S1600536806031229]

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M_r = 429.48
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 16.9257 (16) Å
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c = 16.8911 (15) Å
β = 93.562 (5)°
V = 2144.2 (4) Å^3
Z = 4
$F(000)$ = 912
D_x = 1.330 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4712 reflections
θ = 3.0–27.5°
μ = 0.10 mm^{-1}
T = 120 K
Plate, colourless
0.24 × 0.22 × 0.06 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Radiation source: Bruker-Nonius FR591 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
T_{min} = 0.965, T_{max} = 0.994
23793 measured reflections
4712 independent reflections
3010 reflections with $I > 2\sigma(I)$
R_{int} = 0.067
θ_{max} = 27.5°, θ_{min} = 3.0°
h = −21→21
k = −9→9
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.083
$wR(F^2)$ = 0.222
S = 1.08
4712 reflections
282 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0907P)^2 + 2.3771P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
N11	0.69996 (16)	0.7976 (3)	0.78891 (14)	0.0335 (6)

C12	0.6536 (2)	0.6328 (4)	0.79664 (18)	0.0355 (7)
N13	0.56828 (16)	0.6657 (4)	0.80368 (14)	0.0365 (6)
C14	0.5462 (2)	0.7841 (5)	0.8710 (2)	0.0425 (8)
C15	0.5936 (2)	0.9548 (4)	0.8681 (2)	0.0414 (8)
C16	0.6811 (2)	0.9101 (5)	0.85906 (19)	0.0410 (8)
C21	0.66947 (18)	0.5087 (4)	0.72645 (18)	0.0321 (7)
C22	0.6821 (2)	0.5720 (4)	0.64863 (19)	0.0382 (8)
C23	0.6931 (2)	0.4561 (4)	0.58592 (19)	0.0372 (8)
C24	0.69164 (18)	0.2744 (4)	0.60064 (18)	0.0337 (7)
N24	0.70510 (17)	0.1503 (4)	0.53407 (16)	0.0401 (7)
O21	0.70457 (17)	0.2086 (3)	0.46651 (14)	0.0541 (7)
O22	0.71752 (17)	−0.0070 (3)	0.54932 (15)	0.0554 (7)
C25	0.67844 (19)	0.2069 (4)	0.67673 (18)	0.0361 (8)
C26	0.66765 (19)	0.3263 (4)	0.73860 (19)	0.0360 (7)
C17	0.78529 (19)	0.7628 (4)	0.78205 (18)	0.0371 (8)
C18	0.8327 (2)	0.9140 (4)	0.74341 (18)	0.0369 (8)
C19	0.91819 (19)	0.8602 (4)	0.72293 (18)	0.0361 (8)
N37	0.92010 (16)	0.7556 (4)	0.64971 (14)	0.0349 (6)
C37	0.91861 (18)	0.5874 (4)	0.65696 (17)	0.0326 (7)
C31	0.91118 (18)	0.4678 (4)	0.58863 (18)	0.0314 (7)
C32	0.89958 (19)	0.5339 (4)	0.51321 (18)	0.0363 (8)
C33	0.89443 (19)	0.4196 (4)	0.45034 (18)	0.0364 (8)
C34	0.90149 (19)	0.2380 (4)	0.46366 (18)	0.0352 (7)
N34	0.89963 (17)	0.1166 (4)	0.39599 (16)	0.0413 (7)
O31	0.88460 (16)	0.1784 (3)	0.33098 (14)	0.0533 (7)
O32	0.91459 (16)	−0.0409 (3)	0.40567 (14)	0.0501 (7)
C35	0.91109 (19)	0.1676 (4)	0.53764 (18)	0.0368 (8)
C36	0.9155 (2)	0.2852 (4)	0.60029 (18)	0.0364 (8)
O41	0.48091 (17)	0.3626 (4)	0.83431 (13)	0.0549 (7)
C41	0.4785 (2)	0.3418 (5)	0.91697 (19)	0.0470 (9)
H12	0.6741	0.5718	0.8464	0.043*
H13	0.5565	0.7186	0.7580	0.044*
H14A	0.5579	0.7232	0.9224	0.051*
H14E	0.4889	0.8112	0.8658	0.051*
H15E	0.5882	1.0236	0.9175	0.050*
H15A	0.5732	1.0285	0.8228	0.050*
H16E	0.7106	1.0234	0.8560	0.049*
H16A	0.7016	0.8480	0.9078	0.049*
H22	0.6830	0.6966	0.6393	0.046*
H23	0.7014	0.5003	0.5344	0.045*
H25	0.6769	0.0822	0.6857	0.043*
H26	0.6589	0.2816	0.7899	0.043*
H17A	0.7908	0.6529	0.7505	0.044*
H17B	0.8098	0.7398	0.8358	0.044*
H18A	0.8362	1.0169	0.7801	0.044*
H18B	0.8029	0.9529	0.6941	0.044*
H19A	0.9501	0.9695	0.7174	0.043*
H19B	0.9430	0.7901	0.7675	0.043*

H37	0.9225	0.5374	0.7087	0.039*
H32	0.8951	0.6586	0.5047	0.044*
H33	0.8861	0.4641	0.3978	0.044*
H35	0.9146	0.0427	0.5458	0.044*
H36	0.9217	0.2401	0.6529	0.044*
H41	0.5084	0.4521	0.8246	0.082*
H41A	0.5324	0.3468	0.9416	0.070*
H41B	0.4546	0.2267	0.9285	0.070*
H41C	0.4467	0.4376	0.9383	0.070*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N11	0.0414 (16)	0.0280 (13)	0.0304 (13)	0.0010 (11)	−0.0047 (11)	−0.0028 (11)
C12	0.046 (2)	0.0285 (16)	0.0307 (16)	0.0003 (14)	−0.0052 (14)	0.0003 (13)
N13	0.0436 (17)	0.0369 (15)	0.0283 (13)	−0.0024 (12)	−0.0029 (11)	0.0002 (11)
C14	0.047 (2)	0.042 (2)	0.0385 (18)	0.0011 (16)	0.0017 (15)	−0.0037 (15)
C15	0.051 (2)	0.0357 (18)	0.0363 (18)	0.0028 (16)	−0.0034 (15)	−0.0036 (14)
C16	0.050 (2)	0.0350 (18)	0.0368 (18)	−0.0008 (15)	−0.0076 (15)	−0.0048 (14)
C21	0.0309 (17)	0.0290 (16)	0.0359 (17)	−0.0018 (13)	−0.0030 (13)	−0.0017 (13)
C22	0.046 (2)	0.0283 (16)	0.0392 (18)	−0.0025 (14)	−0.0070 (14)	0.0024 (14)
C23	0.043 (2)	0.0332 (17)	0.0339 (17)	−0.0022 (15)	−0.0069 (14)	0.0041 (14)
C24	0.0312 (17)	0.0337 (17)	0.0352 (17)	0.0004 (14)	−0.0040 (13)	−0.0038 (13)
N24	0.0416 (17)	0.0378 (17)	0.0399 (16)	−0.0021 (13)	−0.0048 (12)	−0.0063 (13)
O21	0.075 (2)	0.0521 (16)	0.0337 (13)	0.0006 (13)	−0.0099 (12)	−0.0052 (11)
O22	0.076 (2)	0.0350 (14)	0.0543 (16)	0.0012 (13)	0.0004 (13)	−0.0072 (12)
C25	0.0399 (19)	0.0288 (17)	0.0390 (18)	−0.0004 (14)	−0.0018 (14)	0.0013 (14)
C26	0.0394 (19)	0.0341 (17)	0.0339 (17)	−0.0003 (14)	−0.0014 (13)	0.0049 (14)
C17	0.043 (2)	0.0350 (17)	0.0316 (16)	0.0015 (15)	−0.0112 (14)	−0.0033 (13)
C18	0.045 (2)	0.0315 (16)	0.0326 (17)	0.0003 (14)	−0.0106 (14)	−0.0031 (13)
C19	0.0416 (19)	0.0299 (17)	0.0355 (17)	−0.0041 (14)	−0.0093 (14)	−0.0013 (13)
N37	0.0375 (16)	0.0334 (14)	0.0328 (14)	−0.0014 (12)	−0.0070 (11)	0.0008 (11)
C37	0.0340 (18)	0.0352 (17)	0.0278 (15)	0.0004 (14)	−0.0048 (12)	0.0014 (13)
C31	0.0293 (17)	0.0317 (16)	0.0326 (16)	−0.0010 (13)	−0.0038 (12)	−0.0002 (13)
C32	0.0424 (19)	0.0315 (17)	0.0341 (17)	0.0024 (14)	−0.0067 (14)	0.0022 (13)
C33	0.0408 (19)	0.0369 (18)	0.0305 (16)	0.0010 (15)	−0.0066 (13)	0.0036 (14)
C34	0.0346 (18)	0.0364 (17)	0.0335 (17)	0.0004 (14)	−0.0062 (13)	−0.0052 (14)
N34	0.0411 (17)	0.0418 (17)	0.0395 (16)	0.0014 (13)	−0.0092 (12)	−0.0057 (13)
O31	0.0747 (19)	0.0465 (15)	0.0362 (13)	0.0094 (13)	−0.0169 (12)	−0.0056 (11)
O32	0.0640 (17)	0.0321 (13)	0.0517 (15)	0.0057 (12)	−0.0165 (12)	−0.0101 (11)
C35	0.0406 (19)	0.0282 (16)	0.0404 (18)	−0.0015 (14)	−0.0070 (14)	0.0013 (14)
C36	0.0420 (19)	0.0351 (18)	0.0311 (16)	0.0023 (14)	−0.0058 (13)	0.0033 (13)
O41	0.0740 (19)	0.0543 (17)	0.0351 (13)	−0.0267 (14)	−0.0079 (12)	0.0017 (11)
C41	0.054 (2)	0.047 (2)	0.0388 (19)	−0.0026 (18)	−0.0050 (16)	0.0022 (16)

Geometric parameters (Å, º)

N11—C12	1.476 (4)	C17—H17A	0.99
N11—C17	1.479 (4)	C17—H17B	0.99
N11—C16	1.506 (4)	C18—C19	1.562 (5)
C12—N13	1.477 (4)	C18—H18A	0.99
C12—C21	1.545 (4)	C18—H18B	0.99
C12—H12	1.00	C19—N37	1.468 (4)
N13—C14	1.509 (4)	C19—H19A	0.99
N13—H13	0.88	C19—H19B	0.99
C14—C15	1.515 (5)	N37—C37	1.270 (4)
C14—H14A	0.99	C37—C31	1.462 (4)
C14—H14E	0.99	C37—H37	0.95
C15—C16	1.535 (5)	C31—C32	1.370 (4)
C15—H15E	0.99	C31—C36	1.387 (4)
C15—H15A	0.99	C32—C33	1.364 (4)
C16—H16E	0.99	C32—H32	0.95
C16—H16A	0.99	C33—C34	1.387 (5)
C21—C26	1.387 (4)	C33—H33	0.95
C21—C22	1.426 (4)	C34—C35	1.357 (4)
C22—C23	1.392 (5)	C34—N34	1.461 (4)
C22—H22	0.95	N34—O31	1.205 (3)
C23—C24	1.389 (4)	N34—O32	1.219 (4)
C23—H23	0.95	C35—C36	1.377 (4)
C24—C25	1.412 (4)	C35—H35	0.95
C24—N24	1.489 (4)	C36—H36	0.95
N24—O21	1.222 (3)	O41—C41	1.408 (4)
N24—O22	1.225 (4)	O41—H41	0.84
C25—C26	1.398 (4)	C41—H41A	0.98
C25—H25	0.95	C41—H41B	0.98
C26—H26	0.95	C41—H41C	0.98
C17—C18	1.557 (5)		
C12—N11—C17	112.7 (2)	N11—C17—C18	115.8 (3)
C12—N11—C16	105.2 (2)	N11—C17—H17A	108.3
C17—N11—C16	114.6 (2)	C18—C17—H17A	108.3
N11—C12—N13	113.2 (2)	N11—C17—H17B	108.3
N11—C12—C21	108.6 (2)	C18—C17—H17B	108.3
N13—C12—C21	112.4 (2)	H17A—C17—H17B	107.4
N11—C12—H12	107.5	C17—C18—C19	114.4 (3)
N13—C12—H12	107.5	C17—C18—H18A	108.7
C21—C12—H12	107.5	C19—C18—H18A	108.7
C12—N13—C14	116.7 (2)	C17—C18—H18B	108.7
C12—N13—H13	100.1	C19—C18—H18B	108.7
C14—N13—H13	109.9	H18A—C18—H18B	107.6
N13—C14—C15	108.5 (3)	N37—C19—C18	113.2 (2)
N13—C14—H14A	110.0	N37—C19—H19A	108.9
C15—C14—H14A	110.0	C18—C19—H19A	108.9

N13—C14—H14E	110.0	N37—C19—H19B	108.9
C15—C14—H14E	110.0	C18—C19—H19B	108.9
H14A—C14—H14E	108.4	H19A—C19—H19B	107.7
C14—C15—C16	109.5 (3)	C37—N37—C19	116.8 (3)
C14—C15—H15E	109.8	N37—C37—C31	122.5 (3)
C16—C15—H15E	109.8	N37—C37—H37	118.8
C14—C15—H15A	109.8	C31—C37—H37	118.8
C16—C15—H15A	109.8	C32—C31—C36	119.6 (3)
H15E—C15—H15A	108.2	C32—C31—C37	120.8 (3)
N11—C16—C15	117.0 (3)	C36—C31—C37	119.6 (3)
N11—C16—H16E	108.0	C33—C32—C31	119.6 (3)
C15—C16—H16E	108.0	C33—C32—H32	120.2
N11—C16—H16A	108.0	C31—C32—H32	120.2
C15—C16—H16A	108.0	C32—C33—C34	119.5 (3)
H16E—C16—H16A	107.3	C32—C33—H33	120.2
C26—C21—C22	118.1 (3)	C34—C33—H33	120.2
C26—C21—C12	118.4 (3)	C35—C34—C33	122.5 (3)
C22—C21—C12	123.3 (3)	C35—C34—N34	118.2 (3)
C23—C22—C21	121.9 (3)	C33—C34—N34	119.3 (3)
C23—C22—H22	119.1	O31—N34—O32	121.8 (3)
C21—C22—H22	119.1	O31—N34—C34	117.8 (3)
C24—C23—C22	118.3 (3)	O32—N34—C34	120.5 (3)
C24—C23—H23	120.9	C34—C35—C36	117.1 (3)
C22—C23—H23	120.9	C34—C35—H35	121.5
C23—C24—C25	121.4 (3)	C36—C35—H35	121.5
C23—C24—N24	118.4 (3)	C35—C36—C31	121.7 (3)
C25—C24—N24	120.2 (3)	C35—C36—H36	119.1
O21—N24—O22	122.2 (3)	C31—C36—H36	119.1
O21—N24—C24	119.2 (3)	C41—O41—H41	109.5
O22—N24—C24	118.5 (3)	O41—C41—H41A	109.5
C26—C25—C24	119.0 (3)	O41—C41—H41B	109.5
C26—C25—H25	120.5	H41A—C41—H41B	109.5
C24—C25—H25	120.5	O41—C41—H41C	109.5
C21—C26—C25	121.2 (3)	H41A—C41—H41C	109.5
C21—C26—H26	119.4	H41B—C41—H41C	109.5
C25—C26—H26	119.4		

C17—N11—C12—N13	179.9 (2)	C22—C21—C26—C25	0.5 (5)
C16—N11—C12—N13	54.4 (3)	C12—C21—C26—C25	177.5 (3)
C17—N11—C12—C21	−54.6 (3)	C24—C25—C26—C21	0.2 (5)
C16—N11—C12—C21	179.9 (2)	C12—N11—C17—C18	158.3 (2)
N11—C12—N13—C14	−57.0 (3)	C16—N11—C17—C18	−81.5 (3)
C21—C12—N13—C14	179.4 (3)	N11—C17—C18—C19	−169.4 (2)
C12—N13—C14—C15	51.6 (4)	C17—C18—C19—N37	78.9 (3)
N13—C14—C15—C16	−48.2 (3)	C18—C19—N37—C37	−92.4 (3)
C12—N11—C16—C15	−57.2 (3)	C19—N37—C37—C31	172.9 (3)
C17—N11—C16—C15	178.5 (3)	N37—C37—C31—C32	−4.9 (5)
C14—C15—C16—N11	56.5 (4)	N37—C37—C31—C36	175.5 (3)

N11—C12—C21—C26	148.1 (3)	C36—C31—C32—C33	−1.6 (5)
N13—C12—C21—C26	−85.9 (3)	C37—C31—C32—C33	178.7 (3)
N11—C12—C21—C22	−35.1 (4)	C31—C32—C33—C34	−0.4 (5)
N13—C12—C21—C22	90.9 (4)	C32—C33—C34—C35	2.0 (5)
C26—C21—C22—C23	−0.5 (5)	C32—C33—C34—N34	−177.2 (3)
C12—C21—C22—C23	−177.4 (3)	C35—C34—N34—O31	174.0 (3)
C21—C22—C23—C24	−0.1 (5)	C33—C34—N34—O31	−6.8 (5)
C22—C23—C24—C25	0.8 (5)	C35—C34—N34—O32	−7.5 (5)
C22—C23—C24—N24	−178.7 (3)	C33—C34—N34—O32	171.7 (3)
C23—C24—N24—O21	−11.4 (4)	C33—C34—C35—C36	−1.5 (5)
C25—C24—N24—O21	169.1 (3)	N34—C34—C35—C36	177.7 (3)
C23—C24—N24—O22	167.5 (3)	C34—C35—C36—C31	−0.6 (5)
C25—C24—N24—O22	−12.0 (4)	C32—C31—C36—C35	2.2 (5)
C23—C24—C25—C26	−0.8 (5)	C37—C31—C36—C35	−178.1 (3)
N24—C24—C25—C26	178.6 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O41—H41···N13	0.84	1.94	2.782 (4)	178
N13—H13···O41^{i}	0.88	1.97	2.841 (3)	171
C17—H17*B*···O32^{ii}	0.99	2.55	3.371 (4)	140
C18—H18*A*···O31^{iii}	0.99	2.56	3.490 (4)	156

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+3/2; (ii) *x*, −*y*+1/2, *z*+1/2; (iii) *x*, −*y*+3/2, *z*+1/2.