**N-(5-Nitropyridin-2-yl)-5H-dibenzo-[d,f][1,3]diazepine-6-carboxamide**

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Received 9 May 2011; accepted 16 May 2011

Key indicators: single-crystal X-ray study; T = 110 K; mean σ(C–C) = 0.001 Å; R factor = 0.036; wR factor = 0.110; data-to-parameter ratio = 18.3.

The title compound, C_{19}H_{13}N_{5}O_{3}, can be obtained from the corresponding α-amido-α-aminonitrone in a reaction with biphenyl-2,2′-diamine. The amido–amine core has distinct geometrical parameters including: an outstandingly long Csp^2–Csp^2 single bond of 1.5276 (13) Å and an amidine N–C–N angle of 130.55 (9)°. Intramolecular N–H···O, N–H···N and C–H···O hydrogen bonds occur. In the crystal, molecules form layers parallel to (001) via weak intermolecular C–H···N interactions. The layers are linked via N–H···O hydrogen bonds and π–π interactions along [001].

**Related literature**

For the synthesis of the title compound, see: Trzewik et al. (2008). For the reaction mechanism, see: Trzewik et al. (2010). For similar structures, see: Zaleska et al. (2007); Hodorowicz et al. (2007). For hydrogen bond graph-set analysis, see: Bernstein et al. (1995).

**Experimental**

Crystal data

| C_{19}H_{13}N_{5}O_{3} | M_r = 359.34 |
|------------------------|-------------|
| monoclinic, P2_1/c | a = 12.9702 (2) Å |
| b = 9.2104 (1) Å | c = 13.4145 (2) Å |
| β = 100.692 (1)° | V = 1574.68 (3) Å^3 |
| Z = 4 | | |
| Mo Kα radiation | μ = 0.11 mm^-1 |
| T = 110 K | 0.30 × 0.20 × 0.15 mm |

**Data collection**

Oxford Diffraction SuperNova
Dual Cu at zero Atlas diffractometer
Absorption correction: multi-scan
(CrysAlis PRO; Oxford, 2009)

Refinement

| R[F^2 > 2σ(F^2)] | 0.036 |
| wR(F^2) | 0.110 |
| S | 1.06 |
| 4577 reflections | 250 parameters |
| 2 restraints | |

H atoms treated by a mixture of independent and constrained refinement

Δρ_{max} = 0.39 e Å^-3
Δρ_{min} = −0.21 e Å^-3

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

| D–H···A | D–H | D···A | D–A | D–H···A |
|---------|------|------|------|---------|
| N2–H2···O4 | 0.89 (1) | 2.24 (1) | 2.7041 (11) | 112 (1) |
| N2–H2···O4' | 0.89 (1) | 2.26 (1) | 3.0725 (11) | 152 (1) |
| N5–H5···N3 | 0.88 (1) | 2.11 (1) | 2.6191 (11) | 156 (1) |
| C55–H55···O4 | 0.95 | 2.33 | 2.9266 (12) | 120 |
| C32–H32···N51 | 0.95 | 2.47 | 3.3000 (13) | 116 |

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

**Data collection:** CrysAlis PRO (Oxford Diffraction, 2009); cell refinement: CrysAlis PRO; program(s) used to solve structure: SIR2004 (Altomare et al., 1994); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: Mercury (Macrae et al., 2006) and ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: SHELXL97, PARST (Nardelli, 1995) and WinGX (Farrugia, 1999).

TS gratefully acknowledges the support from a Project operated within the Foundation for Polish Science MPD Programme co-financed by the EU European Regional Development Fund.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: VM2095).

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N-(5-Nitropyridin-2-yl)-5H-dibenzo[d,f][1,3]diazepine-6-carboxamide

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S1. Comment

The current report is a continuation of an earlier joint theoretical and X-ray study upon the versatile reactivity of $\alpha$-amido-$\alpha$-aminonitrone, having several reactivity centers of different types and yielding various products in reactions with electrophilic and nucleophilic reagents (Trzewik et al., 2008). Among them 5H-dibenzo[d,f][1,3]diazepines, the synthesis and structures of which were described elsewhere (Trzewik et al., 2008, 2010), are unique from the viewpoint of their geometrical features.

The overall shape of the title molecule is shown in Figure 1. The two benzene rings within the diazepine moiety are twisted by torsion angle $C25—C26—C36—C35 = -28.63 (13)^\circ$. The r.m.s. deviation for the best plane through atoms $C21-C26$ is significantly greater than that for $C31-C36$ (0.0166 and 0.0040 Å, respectively) due to steric hindrance between $H25$ and $H35$ ($H25\cdots H35$ distance 2.12 Å).

The puckering parameters of the seven-membered ring (atoms in $C3$, $N2$, $C31$, $C36$, $C26$, $C21$, $N3$ sequence): $q_2 = 0.5324 (9)$, $q_3 = 0.0832 (9)$, $QT = 0.5389 (9)$, $\varphi_2 = 87.6 (1)$, $\varphi_3 = 12.4 (7)$, $\theta_2 = 81.1 (1)^\circ$, indicate a twisted-boat conformation with a pseudo-twofold axis ($C2$) through the $C3$ atom and the centre of $C36—C26$ bond with the deviation of 0.0369 (4) Å, whereas a pseudo-mirror plane (Cs) through $N2$ atom and centre of $C21—C26$ is described by the deviation of 0.0491 (5) Å ($PARST$: Nardelli, 1995).

The rest of the molecule is almost perfectly planar (r.m.s. deviation of fitted atoms equals 0.0181 Å). The fragment of the molecule, relevant from both crystallographic and chemical perspectives, is the amido-amidine core [—N5(—H5)—C4(=O4)—C3(=N3—)—N2(—H2)—]. Within the core distinctive geometrical features of the molecule can be seen: a long $C3(sp^2)—C4(sp^2)$ bond of 1.528 (1) Å and $N2—C3—N3$ angle of 130.55 (9)°. We expect that the planarity of the core moiety possibly results from intramolecular interactions: $N5—H5\cdots N3$, $N2—H2\cdots O4$ and $C55—H55\cdots O4$ (Table 1).

In order to verify the existence of such interactions the analysis of topological properties of electron density distribution is in progress and will be published elsewhere.

The packing of the molecules is organized into layers parallel to (001). Within the layer the molecules are joint by hydrogen bonds of C–H···N type and weak interactions (Figure 2, Table 1). The layers are joined together by $\pi—\pi$ interactions with $Cg1$ ($C31—C36$) and $Cg2$ ($N51—C56$) [-x, $y + 1/2$, -$z + 3/2$] = 3.672 Å (Figure 3); and hydrogen bonds of N —H···O type. The N—H···O hydrogen bond together with its centrosymmetric counterpart form a ring motif with descriptor $R2(10)$ according to graph-set theory (Bernstein et al., 1995). The ring motif is marked in Figure 4.

S2. Experimental

The title compound was synthesized using the procedure already described in literature (Trzewik et al., 2008). Single crystals suitable for X-ray diffraction were grown by slow evaporation from the mixture of methanol and acetonitrile (1:2) solution at ambient conditions.
S3. Refinement

All hydrogen atoms of N—H groups were found in difference Fourier maps and refined in a riding model assuming N—H = 0.88 (2) Å and $U_{iso} = 1.2U_{eq}$ of the parent atom. Aromatic hydrogen atoms were found in difference Fourier maps and refined from geometrical positions assuming C—H = 0.95 Å and using riding model with $U_{iso} = 1.2U_{eq}$.

Figure 1

Asymmetric unit of the title compound showing the atom displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radii.
Figure 2
The hydrogen bond scheme in the layer parallel to (001) cut for $z$ in the range 0.75 to 1.00 (symmetry code: (ii) $x$, $y$-1, $z$).
Figure 3
A diagram of $\pi$—$\pi$ interactions between $Cg_1$ (C31–C36) and $Cg_2^i$ (N51–C56) (symmetry code: (i) $-x, \frac{y}{2}, -z + \frac{3}{2}$).

Figure 4
View of the packing along [001] showing hydrogen bonds between the layers and the ring motif with descriptor $R_2^2(10)$. 
N-(5-Nitropyridin-2-yl)-5H-dibenzo[d,f][1,3]diazepine-6-carboxamide

Crystal data
C_{19}H_{13}N_{5}O_{3}  
$F(000) = 744$

$M_r = 359.34$

Monoclinic, $P2_1/c$

Hall symbol: $-P 2ybc$

$a = 12.9702 (2) \text{ Å}$

$b = 9.2104 (1) \text{ Å}$

$c = 13.4145 (2) \text{ Å}$

$\beta = 100.692 (1)^\circ$

$V = 1574.68 (3) \text{ Å}^3$

$Z = 4$

$F(000) = 744$

$D_x = 1.516 \text{ Mg m}^{-3}$

Melting point = 477–478 K

$\lambda = 0.71073 \text{ Å}$

$\theta = 3.0–44.5^\circ$

$\mu = 0.11 \text{ mm}^{-1}$

$T = 110 \text{ K}$

0.30 × 0.20 × 0.15 mm

Data collection

Oxford Diffraction SuperNova Dual Cu at zero

Atlas diffractometer

Radiation source: Oxford Diffraction SuperNova (Mo) X-ray Source

Mirror monochromator

Detector resolution: 10.3756 pixels mm$^{-1}$

$\omega$ scans

Absorption correction: multi-scan

(CrysAlis PRO; Oxford Diffraction, 2009)

Refinement

Refinement on $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.036$

$wR(F^2) = 0.110$

$S = 1.06$

4577 reflections

250 parameters

2 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: difference Fourier map

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_c^2) + (0.0729P)^2 + 0.1623P]$

where $P = (F_c^2 + 2F_s^2)/3$

$(\Delta\sigma)_{\text{max}} < 0.001$

$\Delta p_{\text{max}} = 0.39 e \text{ Å}^{-3}$

$\Delta p_{\text{min}} = -0.21 e \text{ Å}^{-3}$

Extinction correction: SHELXL97 (Sheldrick, 2008)

Extinction coefficient: 0

Special details

Experimental. CrysAlisPro, Oxford Diffraction Ltd., Version 1.171.33.66. Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm (Oxford Diffraction, 2009).

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 (Å²)

| x       | y       | z       | Uiso*/Ueq |
|---------|---------|---------|-----------|
| N2      | 0.15616 (7) | 0.02467 (9) | 0.92909 (6) | 0.01621 (17) |
| H2      | 0.1014 (9) | −0.0115 (14) | 0.9524 (9) | 0.019* |
| C3      | 0.14265 (7) | 0.16642 (10) | 0.90162 (7) | 0.01300 (18) |
| N3      | 0.20711 (6) | 0.25840 (9) | 0.87513 (6) | 0.01359 (16) |
| C4      | 0.03385 (7) | 0.22423 (10) | 0.90872 (7) | 0.01420 (18) |
| O4      | −0.03207 (5) | 0.14658 (8) | 0.93589 (6) | 0.02028 (17) |
| N5      | 0.02224 (6) | 0.36682 (9) | 0.88352 (6) | 0.01523 (17) |
| H5      | 0.0796 (9) | 0.4033 (13) | 0.8674 (9) | 0.018* |
| C21     | 0.31624 (7) | 0.23319 (10) | 0.88312 (7) | 0.01323 (18) |
| C22     | 0.37511 (8) | 0.36134 (11) | 0.89410 (7) | 0.0173 (2) |
| H22     | 0.3397 | 0.4520 | 0.8913 | 0.021* |
| C23     | 0.48377 (8) | 0.35967 (12) | 0.90890 (8) | 0.0207 (2) |
| H23     | 0.5223 | 0.4479 | 0.9161 | 0.025* |
| C24     | 0.53540 (8) | 0.22716 (12) | 0.91305 (8) | 0.0202 (2) |
| H24     | 0.6099 | 0.2239 | 0.9260 | 0.024* |
| C25     | 0.47790 (7) | 0.09954 (11) | 0.89823 (7) | 0.0172 (2) |
| H25     | 0.5143 | 0.0098 | 0.8995 | 0.021* |
| C26     | 0.36771 (7) | 0.09835 (10) | 0.88136 (7) | 0.01375 (18) |
| C31     | 0.21410 (7) | −0.07550 (10) | 0.88061 (7) | 0.01417 (18) |
| C32     | 0.16788 (8) | −0.21063 (11) | 0.85663 (8) | 0.0187 (2) |
| H32     | 0.1011 | −0.2310 | 0.8730 | 0.022* |
| C33     | 0.21824 (9) | −0.31577 (11) | 0.80897 (8) | 0.0219 (2) |
| H33     | 0.1863 | −0.4078 | 0.7930 | 0.026* |
| C34     | 0.31554 (9) | −0.28566 (11) | 0.78484 (8) | 0.0218 (2) |
| H34     | 0.3509 | −0.3571 | 0.7527 | 0.026* |
| C35     | 0.36072 (8) | −0.15065 (11) | 0.80807 (8) | 0.0181 (2) |
| H35     | 0.4267 | −0.1305 | 0.7900 | 0.022* |
| C36     | 0.31255 (7) | −0.04244 (10) | 0.85732 (7) | 0.01404 (18) |
| N51     | −0.04575 (6) | 0.59431 (9) | 0.85591 (6) | 0.01663 (18) |
| C52     | −0.12294 (8) | 0.69109 (11) | 0.85240 (7) | 0.01701 (19) |
| H52     | −0.1109 | 0.7889 | 0.8352 | 0.020* |
| C53     | −0.21986 (8) | 0.65325 (11) | 0.87304 (7) | 0.01609 (19) |
| C54     | −0.23889 (8) | 0.51174 (11) | 0.90003 (8) | 0.0181 (2) |
| H54     | −0.3054 | 0.4849 | 0.9143 | 0.022* |
| C55     | −0.15953 (7) | 0.41067 (11) | 0.90574 (8) | 0.01687 (19) |
| H55     | −0.1691 | 0.3131 | 0.9251 | 0.020* |
| C56     | −0.06433 (7) | 0.45741 (10) | 0.88190 (7) | 0.01390 (18) |
| N57     | −0.30275 (7) | 0.76288 (10) | 0.86450 (7) | 0.02042 (19) |
| O58     | −0.39181 (6) | 0.72147 (10) | 0.86834 (7) | 0.0296 (2) |
| O59     | −0.27849 (7) | 0.89005 (9) | 0.85351 (7) | 0.02897 (19) |

Atomic displacement parameters (Å²)

| U11   | U22   | U33   | U12   | U13   | U23   |
|-------|-------|-------|-------|-------|-------|
| N2    | 0.0173 (4) | 0.0141 (4) | 0.0190 (4) | 0.0005 (3) | 0.0079 (3) | 0.0029 (3) |

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|   |   |   |   |   |   |
|---|---|---|---|---|---|
| C3 | 0.0147 (4) | 0.0141 (4) | 0.0099 (4) | 0.0007 (3) | 0.0014 (3) | 0.0000 (3) |
| N3 | 0.0138 (4) | 0.0149 (4) | 0.0119 (4) | −0.0002 (3) | 0.0020 (3) | −0.0001 (3) |
| C4 | 0.0150 (4) | 0.0153 (4) | 0.0119 (4) | 0.0004 (3) | 0.0014 (3) | 0.0005 (3) |
| O4 | 0.0173 (3) | 0.0184 (3) | 0.0263 (4) | −0.0001 (3) | 0.0073 (3) | 0.0053 (3) |
| N5 | 0.0124 (4) | 0.0150 (4) | 0.0187 (4) | −0.0001 (3) | 0.0039 (3) | 0.0016 (3) |
| C21 | 0.0137 (4) | 0.0162 (4) | 0.0096 (4) | −0.0006 (3) | 0.0015 (3) | 0.0010 (3) |
| C22 | 0.0191 (5) | 0.0161 (4) | 0.0173 (5) | −0.0019 (3) | 0.0049 (4) | −0.0011 (4) |
| C23 | 0.0189 (5) | 0.0223 (5) | 0.0217 (5) | −0.0066 (4) | 0.0055 (4) | −0.0032 (4) |
| C24 | 0.0138 (4) | 0.0281 (5) | 0.0186 (5) | −0.0021 (4) | 0.0024 (4) | 0.0007 (4) |
| C25 | 0.0154 (4) | 0.0212 (5) | 0.0152 (4) | 0.0021 (4) | 0.0030 (3) | 0.0035 (4) |
| C26 | 0.0156 (4) | 0.0159 (4) | 0.0097 (4) | 0.0004 (3) | 0.0021 (3) | 0.0023 (3) |
| C31 | 0.0161 (4) | 0.0135 (4) | 0.0130 (4) | 0.0018 (3) | 0.0028 (3) | 0.0028 (3) |
| C32 | 0.0199 (5) | 0.0153 (4) | 0.0211 (5) | −0.0014 (4) | 0.0041 (4) | 0.0028 (4) |
| C33 | 0.0280 (5) | 0.0139 (4) | 0.0239 (5) | −0.0009 (4) | 0.0054 (4) | 0.0021 (4) |
| C34 | 0.0294 (5) | 0.0156 (5) | 0.0222 (5) | 0.0044 (4) | 0.0093 (4) | 0.0017 (4) |
| C35 | 0.0197 (4) | 0.0170 (4) | 0.0184 (5) | 0.0039 (4) | 0.0057 (4) | 0.0035 (4) |
| C36 | 0.0155 (4) | 0.0134 (4) | 0.0128 (4) | 0.0015 (3) | 0.0014 (3) | 0.0037 (3) |
| N51 | 0.0172 (4) | 0.0150 (4) | 0.0171 (4) | 0.0001 (3) | 0.0017 (3) | 0.0015 (3) |
| C52 | 0.0201 (4) | 0.0158 (4) | 0.0139 (4) | 0.0010 (4) | −0.0001 (3) | 0.0002 (3) |
| C53 | 0.0168 (4) | 0.0192 (5) | 0.0109 (4) | 0.0048 (3) | −0.0012 (3) | −0.0018 (3) |
| C54 | 0.0146 (4) | 0.0223 (5) | 0.0173 (5) | 0.0006 (4) | 0.0024 (3) | −0.0004 (4) |
| C55 | 0.0151 (4) | 0.0174 (4) | 0.0180 (5) | −0.0011 (3) | 0.0028 (4) | 0.0010 (4) |
| C56 | 0.0142 (4) | 0.0148 (4) | 0.0118 (4) | 0.0006 (3) | 0.0001 (3) | 0.0000 (3) |
| N57 | 0.0221 (4) | 0.0247 (4) | 0.0131 (4) | 0.0081 (3) | −0.0003 (3) | −0.0017 (3) |
| O58 | 0.0187 (4) | 0.0389 (5) | 0.0316 (5) | 0.0099 (3) | 0.0057 (3) | 0.0046 (4) |
| O59 | 0.0345 (5) | 0.0193 (4) | 0.0306 (5) | 0.0084 (3) | −0.0002 (3) | −0.0015 (3) |

**Geometric parameters (Å, °)**

|   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|
| N2—C3 | 1.3591 (12) | C31—C36 | 1.4031 (13) |
| N2—C31 | 1.4213 (12) | C32—C33 | 1.3891 (14) |
| N2—H2 | 0.892 (11) | C32—H32 | 0.9500 |
| C3—N3 | 1.2858 (12) | C33—C34 | 1.3878 (15) |
| C3—C4 | 1.5276 (13) | C33—H33 | 0.9500 |
| N3—C21 | 1.4186 (12) | C34—C35 | 1.3853 (15) |
| C4—O4 | 1.2211 (11) | C34—H34 | 0.9500 |
| C4—N5 | 1.3575 (12) | C35—C36 | 1.4048 (13) |
| N5—C56 | 1.3958 (12) | C35—H35 | 0.9500 |
| N5—H5 | 0.879 (11) | N51—C52 | 1.3348 (13) |
| C21—C22 | 1.3987 (13) | N51—C56 | 1.3419 (12) |
| C21—C26 | 1.4122 (13) | C52—C53 | 1.3812 (14) |
| C22—C23 | 1.3864 (14) | C52—H52 | 0.9500 |
| C22—H22 | 0.9500 | C53—C54 | 1.3870 (14) |
| C23—C24 | 1.3883 (15) | C53—N57 | 1.4639 (13) |
| C23—H23 | 0.9500 | C54—C55 | 1.3794 (13) |
| C24—C25 | 1.3864 (14) | C54—H54 | 0.9500 |
| C24—H24 | 0.9500 | C55—C56 | 1.3996 (13) |
| C25—C26 | 1.4050 (13) | C55—H55 | 0.9500 |
| Bond/Angle | Distance/° | Bond/Distance/° | Distance/° |
|------------|------------|-----------------|------------|
| C25—H25   | 0.9500     | N57—O58         | 1.2265 (12)|
| C26—C36   | 1.4872 (13)| N57—O59         | 1.2288 (13)|
| C31—C32   | 1.3933 (13)|                 |            |
| C3—N2—C31 | 123.51 (8) | C33—C32—C31     | 120.63 (9) |
| C3—N2—H2  | 112.5 (8)  | C33—C32—H32     | 119.7      |
| C31—N2—H2 | 116.2 (8)  | C31—C32—H32     | 119.7      |
| N3—C3—N2  | 130.55 (9) | C34—C33—C32     | 119.62 (10)|
| N3—C3—C4  | 116.30 (8) | C34—C33—H33     | 120.2      |
| N2—C3—C4  | 113.09 (8) | C32—C33—H33     | 120.2      |
| C3—N3—C21 | 124.20 (8) | C35—C34—C33     | 119.47 (9) |
| C3—N5—C51 | 111.8 (8)  | C36—C35—C34     | 120.3      |
| C4—N5—C56 | 118.9 (8)  | C33—C34—C35     | 120.3      |
| C4—N5—H5  | 118.9 (8)  | C31—C34—C35     | 116.95 (9) |
| C56—N5—H5 | 119.56 (8) | C31—C36—C35     | 124.20 (8) |
| C22—C21—C26 | 119.79 (8) | C35—C36—C32     | 118.85 (8) |
| C22—C21—N3 | 127.65 (8) | C52—N51—C56     | 117.84 (8) |
| C23—C22—C21 | 121.75 (9) | N51—C52—C53     | 121.94 (9) |
| C23—C22—H22 | 119.1      | N51—C52—H22     | 119.0      |
| C22—C23—C24 | 119.05 (9) | C53—C52—H22     | 119.0      |
| C22—C23—C24 | 120.5      | C52—C53—C54     | 120.14 (9) |
| C22—C23—H23 | 120.5      | C52—C53—N57     | 119.53 (9) |
| C24—C23—C23 | 119.80 (9) | C54—C53—N57     | 120.33 (9) |
| C24—C23—C24 | 120.1      | C55—C54—C53     | 118.79 (9) |
| C25—C24—C24 | 120.1      | C55—C54—C53     | 120.6      |
| C25—C24—H24 | 122.26 (9) | C54—C55—C56     | 120.6      |
| C24—C25—H24 | 118.9      | C54—C55—C56     | 121.3      |
| C26—C25—H25 | 118.9      | C56—C55—H55     | 121.3      |
| C25—C26—C21 | 117.41 (9) | N51—C56—N5      | 112.52 (8) |
| C25—C26—C36 | 118.41 (8) | N51—C56—C55     | 123.85 (9) |
| C21—C26—C36 | 124.09 (8) | N5—C56—C55      | 123.63 (9) |
| C32—C31—C36 | 120.89 (9) | O58—N57—O59     | 124.44 (9) |
| C32—C31—N2  | 116.34 (8) | O58—N57—C53     | 117.77 (9) |
| C36—C31—N2  | 122.77 (9) | O59—N57—C53     | 117.79 (9) |
| C31—N2—C3—N3 | −40.22 (16)| C32—C33—C34—C35 | −0.43 (16) |
| C31—N2—C3—C4 | 142.83 (9) | C33—C34—C35—C36 | 1.23 (16)  |
| N2—C3—N3—C21 | −9.51 (16) | C32—C31—C36—C35 | 0.77 (14)  |
| C4—C3—N3—C21 | 167.36 (8) | N2—C31—C36—C35 | −179.14 (9) |
| N3—C3—C4—O4 | −177.99 (9) | C32—C31—C36—C26 | −179.29 (9) |
| N2—C3—C4—O4 | −0.58 (13)  | N2—C31—C36—C26  | 0.80 (14)  |
| N3—C3—C4—N5  | 1.05 (12)  | C34—C35—C36—C31 | −1.38 (14) |
| N2—C3—C4—N5  | 178.47 (8) | C34—C35—C36—C26 | 178.68 (9) |
| O4—C4—N5—C56 | −0.22 (17) | C25—C26—C36—C31 | 151.43 (9) |
C3—C4—N5—C56 −179.21 (9) C21—C26—C36—C31 −32.08 (14)
C3—N3—C21—C22 −153.01 (9) C25—C26—C36—C35 −28.63 (13)
C3—N3—C21—C26 26.82 (15) C21—C26—C36—C35 147.86 (9)
C26—C21—C22—C23 −3.56 (15) C56—N51—C52—C53 −0.98 (14)
N3—C21—C22—C23 176.28 (9) N51—C52—C53—C54 1.09 (15)
C21—C22—C23—C24 −0.09 (15) N51—C52—C53—N57 −177.84 (9)
C22—C23—C24—C25 2.66 (15) C52—C53—C54—C55 0.01 (15)
C23—C24—C25—C26 −1.61 (15) C52—N51—C56—N5 −179.63 (8)
C24—C25—C26—C21 −1.98 (14) C52—N51—C56—C55 −0.22 (15)
C24—C25—C26—C36 174.74 (9) C4—N5—C56—N51 177.97 (9)
C22—C21—C26—C25 4.48 (13) C4—N5—C56—C55 −1.44 (16)
N3—C21—C26—C25 −175.34 (9) C54—C55—C56—N51 1.27 (15)
C22—C21—C26—C36 −172.04 (9) C54—C55—C56—N5 −179.39 (9)
N3—C21—C26—C36 8.14 (15) C54—C55—C56—N51 1.27 (15)
C3—N2—C31—C32 −134.33 (10) C54—C55—C56—N5 −179.39 (9)
C3—N2—C31—C36 45.58 (14) C52—C53—N57—O58 169.30 (9)
C36—C31—C32—C33 −0.04 (15) C54—C53—N57—O58 −9.64 (14)
N2—C31—C32—C33 179.87 (10) C52—C53—N57—O59 −10.38 (14)
C31—C32—C33—C34 −0.14 (16) C54—C53—N57—O59 170.68 (9)

Hydrogen-bond geometry (Å, º)

| D—H···A | D—H | H···A | D···A | D—H···A |
|---------|-----|------|-------|---------|
| N2—H2···O4 | 0.89 (1) | 2.24 (1) | 2.7041 (11) | 112 (1) |
| N2—H2···O4i | 0.89 (1) | 2.26 (1) | 3.0725 (11) | 152 (1) |
| N5—H5···N3 | 0.88 (1) | 2.11 (1) | 2.6191 (11) | 116 (1) |
| C55—H55···O4 | 0.95 | 2.33 | 2.9266 (12) | 120 |
| C32—H32···N51i | 0.95 | 2.47 | 3.3000 (13) | 146 |

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