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Ethyl 5-(4-methylphenyl)-2,4,5,7-tetraazatricyclo-[6.4.0.0^{2,6}]dodeca-1(8),3,6,9,11-pentaene-3-carboxylate

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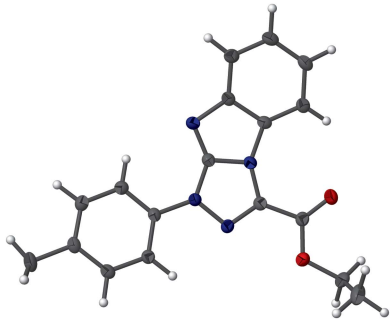
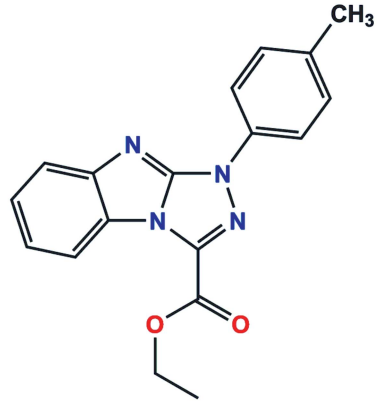
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{18}H_{16}N_4O_2$, the dihedral angle between the fused tricyclic ring system and the pendant benzene ring is 11.03 (4)°. The C—O—C—C torsion angle in the ethyl ester is 102.97 (12)°. The molecular conformation is supported by intramolecular C—H···N and C—H···O hydrogen bonds, which close $S(6)$ and $S(7)$ rings, respectively. Aromatic π–π stacking is observed in the crystal [shortest centroid–centroid separation = 3.5274 (7) Å].

3D view



Chemical scheme



Structure description

As a continuation of our research into benzimidazole derivatives (Moussaif *et al.* 2016, El Bakri *et al.* 2018), the title compound (Fig. 1) was prepared and characterized by single-crystal X-ray diffraction.

The fused tricyclic unit deviates slightly from planarity as indicated by the dihedral angle of 3.87 (6)° between the planes of the C1/C6/N1/C7/N4 and the C7/N2/N3/C8/N4 rings and by the dihedral angle of 2.05 (6)° between the planes of the C1/C6/N1/C7/N4 and the C1–C6 rings. The plane of the pendant C12–C17 ring is inclined to that of the C7/N2/N3/C8/N4 ring by 7.70 (5)°, which is likely due to the combination of the intramolecular C17—H17···N1 hydrogen bond (Table 1 and Fig. 2) and the π-stacking interactions between C7/N2/N3/C8/N4 and C12–C17 rings in inversion-related pairs of molecules [centroid–centroid separation = 3.5274 (7) Å, interplanar angle = 7.70 (5)°]. The orientation of the carboxyl group of the ester substituent is partially determined by the intramolecular C2—H2···O1 hydrogen bond.

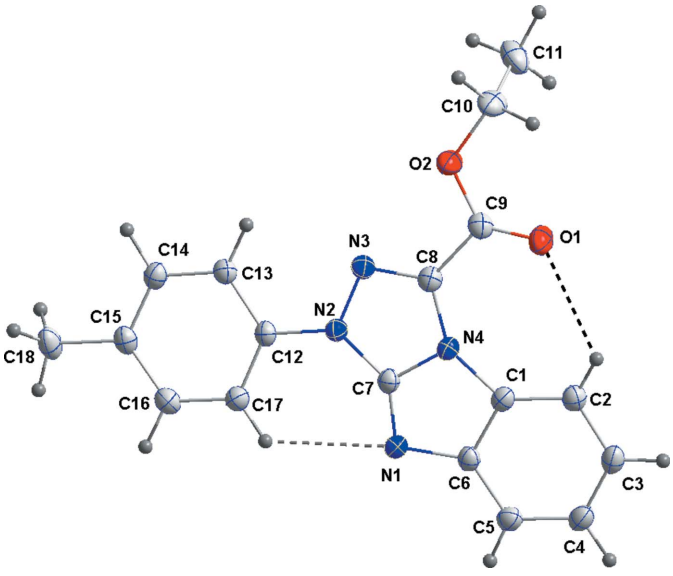


Figure 1
The title molecule with 50% probability ellipsoids. The intramolecular hydrogen bonds are shown as dashed lines.

Synthesis and crystallization

6 mmol of methylmercaptobenzimidazole was dissolved in 40 ml of THF and 8.1 mmol of diphenylnitrileimine and 8.1 mmol of TEA were added. The mixture was refluxed for 24 h using a chilled condenser and $CaCl_2$ trap to minimize water ingress. After cooling, the salts were removed by filtration and the solvent was evaporated under reduced pressure. Light-yellow blocks were obtained by recrystallization from ethanol solution.

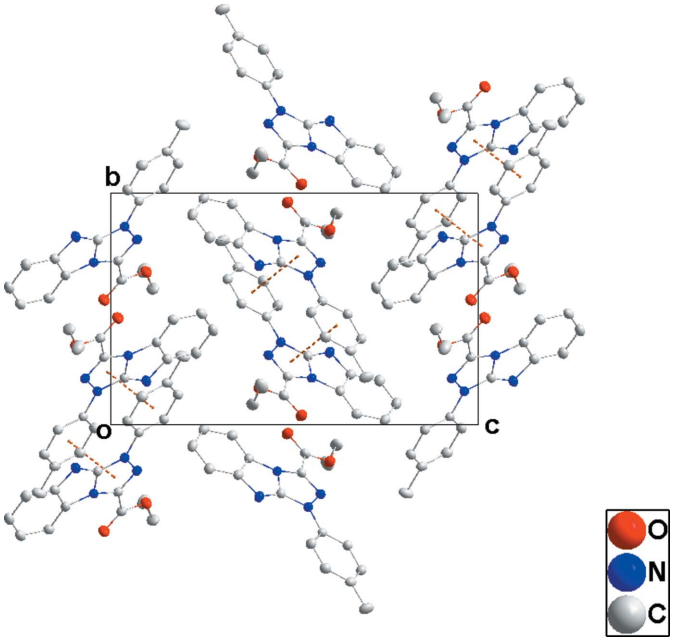


Figure 2
Packing viewed along the *a*-axis direction with π-stacking interactions shown as dashed lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O1	0.941 (14)	2.498 (13)	3.1480 (14)	126.3 (11)
C17—H17···N1	0.956 (13)	2.490 (12)	3.1473 (14)	125.8 (10)

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{16}N_4O_2$
M_r	320.35
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	100
a, b, c (Å)	9.2366 (11), 10.2045 (12), 16.1922 (18)
β (°)	92.144 (2)
V (Å^3)	1525.1 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.10
Crystal size (mm)	0.33 × 0.17 × 0.11
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.88, 0.99
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	28729, 4119, 3269
R_{int}	0.034
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.688
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.044, 0.126, 1.10
No. of reflections	4119
No. of parameters	281
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.43, −0.19

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Funding information

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References

Brandenburg, K. & Putz, H. (2012). *DIAMOND*, Crystal Impact GbR, Bonn, Germany.
Bruker (2016). *APEX3* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
El Bakri, Y., Anouar, E. H., Ramli, Y., Essassi, E. M. & Mague, J. T. (2018). *J. Mol. Struct.* **1152**, 154–162.
Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.
Moussaif, A., Ramli, Y., Sebbar, N. K., Essassi, E. M. & Mague, J. T. (2016). *IUCrData*, **1**, x161948.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

full crystallographic data

IUCrData (2018). **3**, x180892 [https://doi.org/10.1107/S2414314618008921]

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Crystal data

$C_{18}H_{16}N_4O_2$
M_r = 320.35
Monoclinic, $P2_1/n$
a = 9.2366 (11) Å
b = 10.2045 (12) Å
c = 16.1922 (18) Å
β = 92.144 (2)°
V = 1525.1 (3) Å^3
Z = 4
$F(000)$ = 672
D_x = 1.395 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9939 reflections
θ = 2.5–29.2°
μ = 0.10 mm^{-1}
T = 100 K
Column, light yellow
0.33 × 0.17 × 0.11 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min} = 0.88, T_{max} = 0.99
28729 measured reflections
4119 independent reflections
3269 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 29.3°, θ_{min} = 2.4°
h = −12→12
k = −13→14
l = −22→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.126
S = 1.10
4119 reflections
281 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0837P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Special details

Experimental. The diffraction data were obtained from 3 sets of 400 frames, each of width 0.5° in ω, colllected at φ = 0.00, 90.00 and 180.00° and 2 sets of 800 frames, each of width 0.45° in φ, collected at ω = –30.00 and 210.00°. The scan time was 20 sec/frame.

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.

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 $F^2 > 2\text{sigma}(F^2)$ 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*	U_{iso}*/U_{eq}
O1	0.27907 (9)	0.03912 (8)	0.51898 (5)	0.0305 (2)
O2	0.22672 (9)	0.16022 (8)	0.40455 (5)	0.0291 (2)
N1	0.73373 (10)	0.31219 (9)	0.59612 (5)	0.0225 (2)
N2	0.59679 (9)	0.35622 (8)	0.46266 (5)	0.0204 (2)
N3	0.47218 (10)	0.30038 (8)	0.42909 (5)	0.0214 (2)
N4	0.53322 (10)	0.20134 (8)	0.54708 (5)	0.0198 (2)
C1	0.56736 (11)	0.14534 (10)	0.62432 (6)	0.0207 (2)
C2	0.50476 (12)	0.04636 (10)	0.66949 (6)	0.0232 (2)
H2	0.4245 (16)	−0.0026 (14)	0.6496 (8)	0.033 (3)*
C3	0.56831 (12)	0.02072 (11)	0.74701 (7)	0.0260 (2)
H3	0.5272 (15)	−0.0462 (12)	0.7811 (8)	0.029 (3)*
C4	0.68767 (12)	0.09204 (11)	0.77778 (7)	0.0262 (2)
H4	0.7286 (15)	0.0763 (13)	0.8336 (8)	0.031 (3)*
C5	0.75050 (12)	0.19019 (11)	0.73189 (7)	0.0246 (2)
H5	0.8333 (16)	0.2357 (12)	0.7552 (8)	0.035 (4)*
C6	0.69074 (11)	0.21704 (10)	0.65324 (6)	0.0212 (2)
C7	0.63534 (11)	0.29777 (10)	0.53647 (6)	0.0201 (2)
C8	0.43553 (12)	0.20874 (10)	0.48072 (6)	0.0209 (2)
C9	0.30540 (12)	0.12523 (10)	0.47099 (6)	0.0231 (2)
C10	0.09331 (13)	0.08760 (12)	0.38572 (8)	0.0315 (3)
H10A	0.0950 (14)	0.0742 (12)	0.3234 (8)	0.029 (3)*
H10B	0.1026 (15)	−0.0018 (15)	0.4127 (8)	0.041 (4)*
C11	−0.03431 (15)	0.16685 (15)	0.41023 (9)	0.0382 (3)
H11A	−0.0357 (17)	0.1755 (15)	0.4712 (10)	0.049 (4)*
H11B	−0.1280 (16)	0.1198 (14)	0.3897 (8)	0.041 (4)*
H11C	−0.0356 (17)	0.2555 (15)	0.3833 (9)	0.044 (4)*
C12	0.66049 (11)	0.46589 (9)	0.42400 (6)	0.0192 (2)
C13	0.58932 (11)	0.52255 (10)	0.35533 (6)	0.0215 (2)
H13	0.4937 (14)	0.4852 (12)	0.3339 (7)	0.027 (3)*
C14	0.65297 (12)	0.62930 (10)	0.31773 (6)	0.0233 (2)
H14	0.5988 (14)	0.6704 (13)	0.2681 (8)	0.034 (3)*
C15	0.78523 (12)	0.68054 (10)	0.34691 (6)	0.0229 (2)
C16	0.85299 (12)	0.62162 (11)	0.41557 (7)	0.0248 (2)
H16	0.9471 (16)	0.6601 (13)	0.4358 (9)	0.038 (4)*
C17	0.79222 (12)	0.51494 (11)	0.45474 (7)	0.0233 (2)
H17	0.8409 (14)	0.4748 (12)	0.5014 (8)	0.024 (3)*

C18	0.85216 (15)	0.79542 (12)	0.30434 (9)	0.0329 (3)
H18A	0.881 (2)	0.7749 (17)	0.2454 (12)	0.078 (6)*
H18B	0.9384 (18)	0.8226 (15)	0.3336 (9)	0.049 (4)*
H18C	0.786 (2)	0.870 (2)	0.2983 (12)	0.082 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0370 (5)	0.0272 (4)	0.0273 (4)	−0.0104 (3)	−0.0013 (3)	0.0036 (3)
O2	0.0304 (4)	0.0284 (4)	0.0279 (4)	−0.0084 (3)	−0.0064 (3)	0.0036 (3)
N1	0.0221 (5)	0.0253 (5)	0.0199 (4)	−0.0003 (4)	−0.0001 (3)	0.0028 (3)
N2	0.0214 (4)	0.0208 (4)	0.0188 (4)	−0.0022 (3)	−0.0002 (3)	0.0005 (3)
N3	0.0227 (4)	0.0208 (4)	0.0205 (4)	−0.0029 (3)	−0.0003 (3)	−0.0018 (3)
N4	0.0227 (4)	0.0184 (4)	0.0183 (4)	0.0001 (3)	0.0007 (3)	0.0005 (3)
C1	0.0231 (5)	0.0208 (5)	0.0185 (5)	0.0036 (4)	0.0016 (4)	0.0002 (4)
C2	0.0238 (5)	0.0207 (5)	0.0253 (5)	0.0010 (4)	0.0031 (4)	0.0007 (4)
C3	0.0295 (6)	0.0242 (5)	0.0246 (5)	0.0033 (4)	0.0064 (4)	0.0051 (4)
C4	0.0279 (6)	0.0298 (6)	0.0211 (5)	0.0059 (4)	0.0025 (4)	0.0038 (4)
C5	0.0225 (5)	0.0279 (6)	0.0233 (5)	0.0025 (4)	0.0010 (4)	0.0008 (4)
C6	0.0213 (5)	0.0209 (5)	0.0214 (5)	0.0018 (4)	0.0039 (4)	0.0011 (4)
C7	0.0209 (5)	0.0205 (5)	0.0191 (5)	0.0003 (4)	0.0027 (4)	−0.0001 (4)
C8	0.0244 (5)	0.0185 (5)	0.0200 (5)	−0.0005 (4)	0.0014 (4)	−0.0020 (4)
C9	0.0263 (5)	0.0204 (5)	0.0226 (5)	−0.0029 (4)	0.0010 (4)	−0.0032 (4)
C10	0.0337 (6)	0.0284 (6)	0.0317 (6)	−0.0108 (5)	−0.0083 (5)	−0.0022 (5)
C11	0.0339 (7)	0.0448 (8)	0.0365 (7)	−0.0162 (6)	0.0078 (5)	−0.0090 (6)
C12	0.0213 (5)	0.0176 (5)	0.0189 (4)	0.0003 (4)	0.0039 (4)	−0.0011 (4)
C13	0.0226 (5)	0.0207 (5)	0.0211 (5)	−0.0010 (4)	0.0018 (4)	−0.0007 (4)
C14	0.0262 (5)	0.0214 (5)	0.0223 (5)	0.0020 (4)	0.0031 (4)	0.0019 (4)
C15	0.0238 (5)	0.0188 (5)	0.0265 (5)	0.0008 (4)	0.0071 (4)	−0.0009 (4)
C16	0.0214 (5)	0.0245 (5)	0.0285 (5)	−0.0017 (4)	0.0023 (4)	−0.0016 (4)
C17	0.0231 (5)	0.0234 (5)	0.0232 (5)	0.0000 (4)	−0.0001 (4)	0.0010 (4)
C18	0.0297 (6)	0.0251 (6)	0.0447 (7)	−0.0028 (5)	0.0096 (5)	0.0079 (5)

Geometric parameters (Å, º)

O1—C9	1.2038 (13)	C8—C9	1.4770 (15)
O2—C9	1.3246 (13)	C10—C11	1.4953 (19)
O2—C10	1.4603 (13)	C10—H10A	1.019 (13)
N1—C7	1.3094 (13)	C10—H10B	1.014 (15)
N1—C6	1.4083 (13)	C11—H11A	0.992 (16)
N2—C7	1.3709 (12)	C11—H11B	1.034 (15)
N2—N3	1.3777 (12)	C11—H11C	1.004 (15)
N2—C12	1.4207 (13)	C12—C17	1.3905 (15)
N3—C8	1.3072 (13)	C12—C13	1.3957 (14)
N4—C7	1.3783 (14)	C13—C14	1.3891 (14)
N4—C8	1.3791 (13)	C13—H13	1.011 (13)
N4—C1	1.4002 (12)	C14—C15	1.3950 (15)
C1—C2	1.3860 (14)	C14—H14	1.020 (13)

C1—C6	1.4190 (14)	C15—C16	1.3918 (15)
C2—C3	1.3905 (15)	C15—C18	1.5045 (15)
C2—H2	0.941 (14)	C16—C17	1.3889 (15)
C3—C4	1.3973 (17)	C16—H16	0.999 (14)
C3—H3	0.965 (12)	C17—H17	0.956 (13)
C4—C5	1.3872 (16)	C18—H18A	1.021 (19)
C4—H4	0.980 (14)	C18—H18B	0.952 (17)
C5—C6	1.3961 (14)	C18—H18C	0.98 (2)
C5—H5	0.960 (15)		

C9—O2—C10	117.77 (9)	O2—C10—C11	109.73 (10)
C7—N1—C6	101.65 (9)	O2—C10—H10A	103.4 (7)
C7—N2—N3	110.48 (8)	C11—C10—H10A	112.1 (7)
C7—N2—C12	128.95 (8)	O2—C10—H10B	108.0 (8)
N3—N2—C12	120.37 (8)	C11—C10—H10B	115.3 (8)
C8—N3—N2	106.03 (8)	H10A—C10—H10B	107.5 (11)
C7—N4—C8	107.14 (8)	C10—C11—H11A	110.6 (9)
C7—N4—C1	105.68 (9)	C10—C11—H11B	108.8 (8)
C8—N4—C1	146.85 (9)	H11A—C11—H11B	108.6 (12)
C2—C1—N4	133.18 (10)	C10—C11—H11C	111.6 (9)
C2—C1—C6	123.18 (9)	H11A—C11—H11C	110.6 (12)
N4—C1—C6	103.63 (9)	H11B—C11—H11C	106.4 (12)
C1—C2—C3	116.31 (10)	C17—C12—C13	121.06 (9)
C1—C2—H2	123.0 (8)	C17—C12—N2	119.81 (9)
C3—C2—H2	120.7 (8)	C13—C12—N2	119.14 (9)
C2—C3—C4	121.64 (10)	C14—C13—C12	118.66 (10)
C2—C3—H3	119.2 (8)	C14—C13—H13	121.6 (7)
C4—C3—H3	119.1 (8)	C12—C13—H13	119.7 (7)
C5—C4—C3	121.70 (10)	C13—C14—C15	121.67 (10)
C5—C4—H4	117.3 (8)	C13—C14—H14	117.6 (8)
C3—C4—H4	121.0 (8)	C15—C14—H14	120.7 (8)
C4—C5—C6	118.12 (10)	C16—C15—C14	118.07 (10)
C4—C5—H5	118.8 (8)	C16—C15—C18	121.49 (10)
C6—C5—H5	123.1 (8)	C14—C15—C18	120.43 (10)
C5—C6—N1	128.52 (10)	C17—C16—C15	121.74 (10)
C5—C6—C1	119.02 (10)	C17—C16—H16	121.4 (8)
N1—C6—C1	112.43 (9)	C15—C16—H16	116.9 (8)
N1—C7—N2	138.13 (10)	C16—C17—C12	118.80 (10)
N1—C7—N4	116.59 (9)	C16—C17—H17	120.7 (8)
N2—C7—N4	105.22 (9)	C12—C17—H17	120.5 (8)
N3—C8—N4	111.10 (9)	C15—C18—H18A	113.1 (10)
N3—C8—C9	125.01 (9)	C15—C18—H18B	110.4 (9)
N4—C8—C9	123.88 (9)	H18A—C18—H18B	106.6 (14)
O1—C9—O2	127.09 (10)	C15—C18—H18C	112.8 (12)
O1—C9—C8	122.38 (10)	H18A—C18—H18C	104.3 (15)
O2—C9—C8	110.53 (9)	H18B—C18—H18C	109.3 (14)

C7—N2—N3—C8	−0.56 (11)	C1—N4—C7—N2	−177.11 (8)

C12—N2—N3—C8	−175.94 (8)	N2—N3—C8—N4	−0.66 (12)
C7—N4—C1—C2	179.09 (11)	N2—N3—C8—C9	178.15 (9)
C8—N4—C1—C2	7.4 (2)	C7—N4—C8—N3	1.62 (12)
C7—N4—C1—C6	0.22 (10)	C1—N4—C8—N3	173.26 (13)
C8—N4—C1—C6	−171.48 (14)	C7—N4—C8—C9	−177.21 (9)
N4—C1—C2—C3	−177.77 (10)	C1—N4—C8—C9	−5.6 (2)
C6—C1—C2—C3	0.92 (15)	C10—O2—C9—O1	−0.36 (17)
C1—C2—C3—C4	0.69 (16)	C10—O2—C9—C8	−179.86 (9)
C2—C3—C4—C5	−1.30 (17)	N3—C8—C9—O1	177.45 (10)
C3—C4—C5—C6	0.26 (16)	N4—C8—C9—O1	−3.88 (17)
C4—C5—C6—N1	179.03 (10)	N3—C8—C9—O2	−3.03 (15)
C4—C5—C6—C1	1.28 (15)	N4—C8—C9—O2	175.64 (10)
C7—N1—C6—C5	−176.48 (11)	C9—O2—C10—C11	102.97 (12)
C7—N1—C6—C1	1.39 (11)	C7—N2—C12—C17	10.61 (16)
C2—C1—C6—C5	−1.94 (16)	N3—N2—C12—C17	−174.96 (9)
N4—C1—C6—C5	177.08 (9)	C7—N2—C12—C13	−169.52 (9)
C2—C1—C6—N1	179.97 (9)	N3—N2—C12—C13	4.91 (14)
N4—C1—C6—N1	−1.02 (11)	C17—C12—C13—C14	0.22 (15)
C6—N1—C7—N2	175.57 (12)	N2—C12—C13—C14	−179.65 (9)
C6—N1—C7—N4	−1.28 (12)	C12—C13—C14—C15	−0.02 (16)
N3—N2—C7—N1	−175.57 (12)	C13—C14—C15—C16	−0.06 (16)
C12—N2—C7—N1	−0.7 (2)	C13—C14—C15—C18	179.39 (10)
N3—N2—C7—N4	1.52 (11)	C14—C15—C16—C17	−0.07 (16)
C12—N2—C7—N4	176.39 (9)	C18—C15—C16—C17	−179.52 (11)
C8—N4—C7—N1	175.98 (9)	C15—C16—C17—C12	0.28 (16)
C1—N4—C7—N1	0.72 (12)	C13—C12—C17—C16	−0.35 (16)
C8—N4—C7—N2	−1.85 (11)	N2—C12—C17—C16	179.52 (9)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O1	0.941 (14)	2.498 (13)	3.1480 (14)	126.3 (11)
C17—H17···N1	0.956 (13)	2.490 (12)	3.1473 (14)	125.8 (10)