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4-[5-(Benzofuran-2-yl)-1-phenyl-1*H*-pyrazol-3-yl]-*N*,*N*-dimethylaniline

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Keywords: crystal structure; benzofuran derivative; π–π stacking; inversion dimers.

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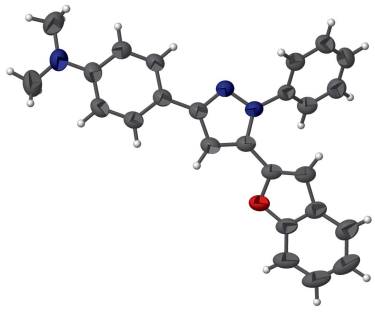
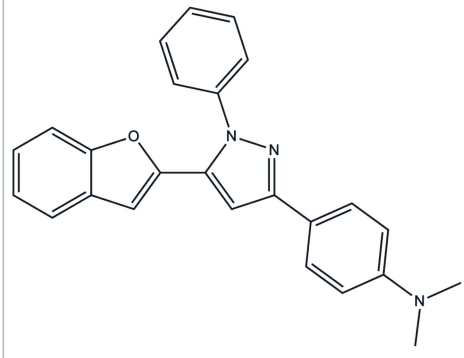
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{25}H_{21}N_3O$, the dihedral angles between the pyrazole ring and its phenyl, aniline and benzofuran (r.m.s. deviation = 0.006 Å) substituents are 47.64 (8), 4.00 (8) and 29.12 (7)°, respectively. The methyl C atoms of the aniline group deviate from their attached ring by 0.521 (3) and 0.010 (3) Å. In the crystal, aromatic π–π stacking between the pyrazole rings [centroid–centroid separation = 3.7899 (9) Å and slippage = 0.66 Å] generates inversion dimers.

3D view



Chemical scheme



Structure description

Benzofuran derivatives are found in many natural bioactive compounds (Khanam & Shamsuzzaman, 2015). In this paper, we report the synthesis and crystal structure of the title benzofuran-pyrazole hybrid.

In the molecular structure of the title compound (Fig. 1), the pyrazole ring makes dihedral angles of 29.12 (7) and 47.64 (8)° withe the phenyl ring (C20–C25) and the mean plane of the benzofuran ring system (O1/C12–C19), respectively. The pyrazole ring is almost coplanar with the benzene ring (C4–C9), as indicated by the dihedral angle of 4.00 (8)°. The methyl C atoms of the aniline group deviate from their attached ring by 0.521 (3) and 0.010 (3) Å. In the crystal, aromatic π–π stacking between the pyrazole rings [centroid–centroid separation = 3.7899 (9); slippage = 0.66 Å) generates inversion dimers.

Synthesis and crystallization

A solution of 1-(benzofuran-2-yl)-3-(4-(dimethylamino)phenyl)-3-thioxopropan-1-one (0.81 g, 2.5 mmol, 1.0 eq.) and phenylhydrazine (0.40 g, 3.75 mmol, 1.5 eq.) in ethanol

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{25}H_{21}N_3O$
M_r	379.45
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	9.6600 (8), 14.9306 (13), 14.5976 (13)
β (°)	107.832 (3)
V (Å^3)	2004.3 (3)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.62
Crystal size (mm)	0.27 × 0.26 × 0.22
Data collection	
Diffractometer	Bruker X8 Proteum
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.851, 0.877
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	17500, 3298, 3063
R_{int}	0.042
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.586
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.048, 0.135, 1.06
No. of reflections	3298
No. of parameters	265
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.23, −0.19

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

(10 ml) was refluxed for 3 h. The course of the reaction was monitored by thin-layer chromatography (TLC). After completion, the solvent was removed under reduced pressure, then the residue was extracted with ethyl acetate. The combined ethyl acetate layers were dried over anhydrous magnesium sulfate, filtered and the solvent removed under reduced pressure to afford the crude product which was purified by column chromatography using silica gel of mesh size 60–120 using an eluent mixture of ethyl acetate and hexane (ratio 2:8). Finally, the title compound was crystallized as colourless blocks from a solvent mixture of ethyl acetate/hexane (yield 77%, m.p. 178–180 K).

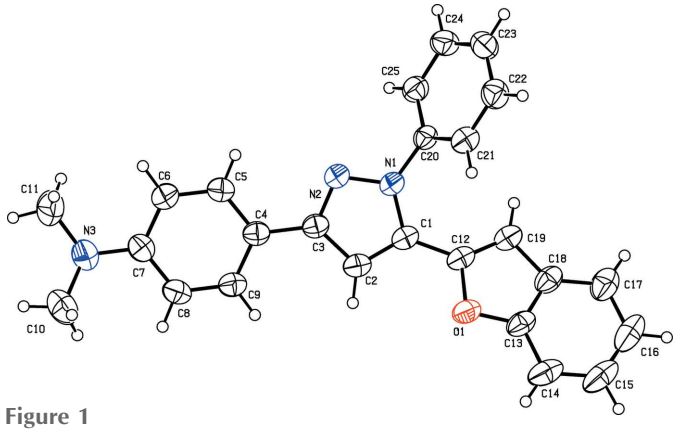


Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x161360 [doi:10.1107/S2414314616013602]

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Crystal data

$C_{25}H_{21}N_3O$
M_r = 379.45
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 9.6600 (8) Å
b = 14.9306 (13) Å
c = 14.5976 (13) Å
β = 107.832 (3)°
V = 2004.3 (3) Å^3
Z = 4
$F(000)$ = 800
D_x = 1.258 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 3298 reflections
θ = 6.4–64.6°
μ = 0.62 mm^{-1}
T = 296 K
Block, colourless
0.27 × 0.26 × 0.22 mm

Data collection

Bruker X8 Proteum diffractometer
Radiation source: Bruker MicroStar microfocus rotating anode
Helios multilayer optics monochromator
Detector resolution: 10.7 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2009)
T_{min} = 0.851, T_{max} = 0.877
17500 measured reflections
3298 independent reflections
3063 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 64.6°, θ_{min} = 6.4°
h = −11→11
k = −17→17
l = −15→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.135
S = 1.06
3298 reflections
265 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
$w = 1/[\sigma^2(F_o^2) + (0.0787P)^2 + 0.3177P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Extinction correction: SHELXL97 (Sheldrick, 2008), $FC^*=KFC[1+0.001XFC^2\Lambda^3/SIN(2\Theta)]^{-1/4}$
Extinction coefficient: 0.0131 (13)

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs 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	0.30155 (11)	0.72252 (7)	0.33607 (8)	0.0575 (4)
N1	0.64307 (13)	0.61185 (8)	0.45780 (9)	0.0490 (4)
N2	0.69905 (13)	0.59191 (8)	0.55309 (9)	0.0505 (4)
N3	0.68633 (17)	0.56415 (13)	0.99273 (11)	0.0744 (6)
C1	0.50112 (15)	0.63863 (9)	0.43519 (11)	0.0488 (4)
C2	0.46516 (16)	0.63547 (10)	0.51835 (12)	0.0527 (5)
C3	0.59079 (16)	0.60660 (9)	0.59031 (11)	0.0485 (4)
C4	0.61425 (16)	0.59408 (9)	0.69352 (11)	0.0491 (5)
C5	0.74975 (17)	0.57019 (11)	0.75589 (12)	0.0571 (5)
C6	0.77438 (18)	0.56078 (12)	0.85328 (12)	0.0613 (5)
C7	0.66317 (19)	0.57498 (11)	0.89460 (12)	0.0573 (5)
C8	0.52667 (19)	0.59812 (11)	0.83193 (12)	0.0588 (5)
C9	0.50328 (17)	0.60728 (10)	0.73467 (12)	0.0545 (5)
C10	0.5955 (3)	0.6120 (2)	1.03840 (17)	0.1018 (11)
C11	0.8309 (2)	0.54142 (18)	1.05430 (14)	0.0906 (8)
C12	0.41158 (15)	0.66189 (10)	0.33844 (11)	0.0504 (4)
C13	0.22834 (16)	0.73479 (10)	0.24000 (12)	0.0570 (5)
C14	0.11052 (19)	0.79098 (13)	0.20348 (17)	0.0768 (7)
C15	0.0528 (2)	0.79331 (16)	0.10493 (19)	0.0887 (8)
C16	0.1111 (2)	0.74309 (17)	0.04622 (17)	0.0891 (8)
C17	0.2296 (2)	0.68770 (14)	0.08376 (14)	0.0748 (7)
C18	0.28960 (16)	0.68347 (11)	0.18382 (12)	0.0560 (5)
C19	0.40827 (17)	0.63671 (11)	0.25015 (12)	0.0564 (5)
C20	0.74029 (15)	0.61106 (10)	0.40139 (10)	0.0472 (4)
C21	0.74874 (17)	0.68401 (11)	0.34471 (12)	0.0575 (5)
C22	0.84898 (19)	0.68341 (12)	0.29489 (13)	0.0648 (6)
C23	0.94310 (19)	0.61256 (13)	0.30358 (12)	0.0645 (6)
C24	0.93492 (18)	0.54034 (12)	0.36047 (12)	0.0635 (6)
C25	0.83201 (17)	0.53859 (11)	0.40866 (11)	0.0554 (5)
H2	0.37560	0.64960	0.52600	0.0630*
H5	0.82610	0.56030	0.73080	0.0690*
H6	0.86650	0.54470	0.89240	0.0740*
H8	0.44990	0.60750	0.85670	0.0710*
H9	0.41100	0.62270	0.69530	0.0650*
H10A	0.61000	0.67520	1.03400	0.1530*
H10B	0.62070	0.59480	1.10490	0.1530*
H10C	0.49530	0.59760	1.00680	0.1530*
H11A	0.86730	0.49130	1.02740	0.1360*
H11B	0.82660	0.52610	1.11720	0.1360*

H11C	0.89440	0.59180	1.05900	0.1360*
H14	0.07250	0.82520	0.24330	0.0920*
H15	−0.02740	0.82960	0.07710	0.1060*
H16	0.06950	0.74660	−0.02020	0.1070*
H17	0.26820	0.65430	0.04370	0.0900*
H19	0.47100	0.59650	0.23450	0.0680*
H21	0.68740	0.73290	0.34030	0.0690*
H22	0.85300	0.73130	0.25510	0.0780*
H23	1.01220	0.61340	0.27110	0.0770*
H24	0.99890	0.49260	0.36650	0.0760*
H25	0.82460	0.48910	0.44560	0.0660*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0438 (6)	0.0580 (6)	0.0693 (7)	0.0088 (4)	0.0151 (5)	0.0108 (5)
N1	0.0407 (6)	0.0544 (7)	0.0485 (7)	0.0045 (5)	0.0087 (5)	0.0034 (5)
N2	0.0442 (6)	0.0556 (7)	0.0496 (7)	0.0042 (5)	0.0111 (5)	0.0028 (5)
N3	0.0762 (10)	0.0937 (11)	0.0555 (8)	0.0022 (8)	0.0236 (7)	−0.0031 (7)
C1	0.0406 (7)	0.0445 (7)	0.0579 (9)	0.0018 (6)	0.0099 (6)	0.0030 (6)
C2	0.0426 (8)	0.0514 (8)	0.0638 (9)	0.0037 (6)	0.0159 (7)	0.0027 (7)
C3	0.0460 (8)	0.0427 (7)	0.0563 (8)	0.0008 (6)	0.0149 (7)	0.0007 (6)
C4	0.0477 (8)	0.0423 (7)	0.0581 (9)	0.0010 (6)	0.0172 (7)	0.0001 (6)
C5	0.0470 (8)	0.0673 (10)	0.0592 (9)	0.0034 (7)	0.0195 (7)	0.0000 (7)
C6	0.0492 (8)	0.0735 (10)	0.0582 (9)	0.0029 (8)	0.0121 (7)	0.0024 (8)
C7	0.0625 (9)	0.0558 (9)	0.0567 (9)	−0.0027 (7)	0.0227 (8)	−0.0034 (7)
C8	0.0571 (9)	0.0588 (9)	0.0678 (10)	0.0050 (7)	0.0301 (8)	−0.0008 (7)
C9	0.0491 (8)	0.0510 (8)	0.0640 (10)	0.0061 (6)	0.0184 (7)	0.0020 (7)
C10	0.123 (2)	0.121 (2)	0.0741 (14)	0.0178 (16)	0.0490 (14)	−0.0075 (13)
C11	0.0872 (14)	0.1205 (18)	0.0563 (11)	−0.0023 (13)	0.0105 (10)	−0.0008 (11)
C12	0.0383 (7)	0.0450 (7)	0.0632 (9)	0.0029 (6)	0.0085 (6)	0.0068 (6)
C13	0.0387 (7)	0.0545 (9)	0.0725 (10)	−0.0014 (6)	0.0094 (7)	0.0188 (7)
C14	0.0480 (9)	0.0678 (11)	0.1079 (16)	0.0106 (8)	0.0142 (9)	0.0262 (10)
C15	0.0556 (11)	0.0802 (13)	0.1105 (17)	0.0051 (10)	−0.0038 (11)	0.0389 (13)
C16	0.0684 (12)	0.0938 (15)	0.0817 (13)	−0.0118 (11)	−0.0118 (11)	0.0356 (12)
C17	0.0642 (11)	0.0815 (12)	0.0674 (11)	−0.0074 (9)	0.0035 (9)	0.0099 (9)
C18	0.0425 (8)	0.0537 (8)	0.0641 (9)	−0.0065 (6)	0.0049 (7)	0.0109 (7)
C19	0.0465 (8)	0.0540 (9)	0.0621 (9)	0.0066 (6)	0.0069 (7)	0.0020 (7)
C20	0.0397 (7)	0.0532 (8)	0.0443 (7)	−0.0005 (6)	0.0064 (6)	−0.0022 (6)
C21	0.0513 (8)	0.0533 (8)	0.0643 (9)	0.0009 (7)	0.0126 (7)	0.0042 (7)
C22	0.0639 (10)	0.0680 (10)	0.0631 (10)	−0.0070 (8)	0.0204 (8)	0.0071 (8)
C23	0.0596 (10)	0.0790 (11)	0.0587 (10)	−0.0065 (8)	0.0238 (8)	−0.0087 (8)
C24	0.0587 (9)	0.0687 (10)	0.0641 (10)	0.0099 (8)	0.0205 (8)	−0.0068 (8)
C25	0.0546 (8)	0.0551 (9)	0.0543 (8)	0.0051 (7)	0.0134 (7)	0.0014 (7)

Geometric parameters (Å, º)

O1—C12	1.3885 (19)	C20—C21	1.385 (2)
O1—C13	1.376 (2)	C20—C25	1.382 (2)
N1—N2	1.3621 (18)	C21—C22	1.378 (3)
N1—C1	1.368 (2)	C22—C23	1.375 (3)
N1—C20	1.426 (2)	C23—C24	1.378 (3)
N2—C3	1.336 (2)	C24—C25	1.383 (2)
N3—C7	1.390 (2)	C2—H2	0.9300
N3—C10	1.443 (3)	C5—H5	0.9300
N3—C11	1.451 (3)	C6—H6	0.9300
C1—C2	1.362 (2)	C8—H8	0.9300
C1—C12	1.454 (2)	C9—H9	0.9300
C2—C3	1.408 (2)	C10—H10A	0.9600
C3—C4	1.465 (2)	C10—H10B	0.9600
C4—C5	1.393 (2)	C10—H10C	0.9600
C4—C9	1.394 (2)	C11—H11A	0.9600
C5—C6	1.375 (2)	C11—H11B	0.9600
C6—C7	1.400 (3)	C11—H11C	0.9600
C7—C8	1.399 (3)	C14—H14	0.9300
C8—C9	1.374 (2)	C15—H15	0.9300
C12—C19	1.334 (2)	C16—H16	0.9300
C13—C14	1.383 (3)	C17—H17	0.9300
C13—C18	1.381 (2)	C19—H19	0.9300
C14—C15	1.375 (4)	C21—H21	0.9300
C15—C16	1.382 (3)	C22—H22	0.9300
C16—C17	1.382 (3)	C23—H23	0.9300
C17—C18	1.398 (3)	C24—H24	0.9300
C18—C19	1.435 (2)	C25—H25	0.9300
C12—O1—C13	105.24 (12)	C23—C24—C25	120.28 (17)
N2—N1—C1	111.43 (12)	C20—C25—C24	119.35 (15)
N2—N1—C20	117.53 (12)	C1—C2—H2	127.00
C1—N1—C20	130.67 (13)	C3—C2—H2	127.00
N1—N2—C3	105.31 (12)	C4—C5—H5	119.00
C7—N3—C10	119.32 (17)	C6—C5—H5	119.00
C7—N3—C11	119.10 (16)	C5—C6—H6	119.00
C10—N3—C11	115.83 (17)	C7—C6—H6	119.00
N1—C1—C2	106.57 (13)	C7—C8—H8	119.00
N1—C1—C12	123.93 (14)	C9—C8—H8	119.00
C2—C1—C12	129.47 (14)	C4—C9—H9	119.00
C1—C2—C3	106.19 (14)	C8—C9—H9	119.00
N2—C3—C2	110.50 (14)	N3—C10—H10A	110.00
N2—C3—C4	120.22 (14)	N3—C10—H10B	109.00
C2—C3—C4	129.27 (15)	N3—C10—H10C	109.00
C3—C4—C5	121.56 (15)	H10A—C10—H10B	109.00
C3—C4—C9	121.86 (14)	H10A—C10—H10C	110.00
C5—C4—C9	116.57 (14)	H10B—C10—H10C	109.00

C4—C5—C6	122.18 (16)	N3—C11—H11A	109.00
C5—C6—C7	121.16 (16)	N3—C11—H11B	109.00
N3—C7—C6	121.59 (16)	N3—C11—H11C	110.00
N3—C7—C8	121.66 (17)	H11A—C11—H11B	110.00
C6—C7—C8	116.73 (15)	H11A—C11—H11C	110.00
C7—C8—C9	121.61 (17)	H11B—C11—H11C	109.00
C4—C9—C8	121.75 (16)	C13—C14—H14	122.00
O1—C12—C1	113.76 (13)	C15—C14—H14	122.00
O1—C12—C19	111.60 (14)	C14—C15—H15	119.00
C1—C12—C19	134.62 (15)	C16—C15—H15	119.00
O1—C13—C14	125.40 (16)	C15—C16—H16	119.00
O1—C13—C18	110.58 (14)	C17—C16—H16	119.00
C14—C13—C18	124.02 (17)	C16—C17—H17	121.00
C13—C14—C15	116.17 (19)	C18—C17—H17	121.00
C14—C15—C16	121.6 (2)	C12—C19—H19	127.00
C15—C16—C17	121.6 (2)	C18—C19—H19	126.00
C16—C17—C18	117.99 (19)	C20—C21—H21	120.00
C13—C18—C17	118.65 (16)	C22—C21—H21	120.00
C13—C18—C19	105.56 (14)	C21—C22—H22	120.00
C17—C18—C19	135.79 (16)	C23—C22—H22	120.00
C12—C19—C18	107.02 (15)	C22—C23—H23	120.00
N1—C20—C21	120.53 (14)	C24—C23—H23	120.00
N1—C20—C25	118.83 (13)	C23—C24—H24	120.00
C21—C20—C25	120.52 (14)	C25—C24—H24	120.00
C20—C21—C22	119.32 (15)	C20—C25—H25	120.00
C21—C22—C23	120.53 (17)	C24—C25—H25	120.00
C22—C23—C24	119.95 (17)		

C13—O1—C12—C1	−178.98 (12)	C9—C4—C5—C6	−0.6 (2)
C13—O1—C12—C19	−0.42 (17)	C3—C4—C9—C8	−178.01 (14)
C12—O1—C13—C14	−179.22 (16)	C5—C4—C9—C8	0.7 (2)
C12—O1—C13—C18	0.24 (17)	C4—C5—C6—C7	0.0 (3)
C1—N1—N2—C3	−0.12 (15)	C5—C6—C7—N3	178.89 (17)
C20—N1—N2—C3	173.62 (12)	C5—C6—C7—C8	0.6 (3)
N2—N1—C1—C2	−0.18 (16)	N3—C7—C8—C9	−178.84 (16)
N2—N1—C1—C12	−178.26 (13)	C6—C7—C8—C9	−0.6 (2)
C20—N1—C1—C2	−172.85 (14)	C7—C8—C9—C4	−0.1 (2)
C20—N1—C1—C12	9.1 (2)	O1—C12—C19—C18	0.42 (18)
N2—N1—C20—C21	−127.92 (15)	C1—C12—C19—C18	178.58 (17)
N2—N1—C20—C25	48.26 (19)	O1—C13—C14—C15	−179.84 (17)
C1—N1—C20—C21	44.4 (2)	C18—C13—C14—C15	0.8 (3)
C1—N1—C20—C25	−139.44 (16)	O1—C13—C18—C17	−179.69 (15)
N1—N2—C3—C2	0.36 (15)	O1—C13—C18—C19	0.0 (2)
N1—N2—C3—C4	−178.30 (12)	C14—C13—C18—C17	−0.2 (3)
C10—N3—C7—C6	154.9 (2)	C14—C13—C18—C19	179.47 (16)
C10—N3—C7—C8	−26.9 (3)	C13—C14—C15—C16	−0.9 (3)
C11—N3—C7—C6	2.8 (3)	C14—C15—C16—C17	0.4 (4)
C11—N3—C7—C8	−179.09 (19)	C15—C16—C17—C18	0.2 (3)

N1—C1—C2—C3	0.39 (16)	C16—C17—C18—C13	−0.3 (3)
C12—C1—C2—C3	178.32 (14)	C16—C17—C18—C19	−179.8 (2)
N1—C1—C12—O1	−152.67 (13)	C13—C18—C19—C12	−0.25 (18)
N1—C1—C12—C19	29.2 (3)	C17—C18—C19—C12	179.4 (2)
C2—C1—C12—O1	29.7 (2)	N1—C20—C21—C22	176.61 (15)
C2—C1—C12—C19	−148.41 (19)	C25—C20—C21—C22	0.5 (2)
C1—C2—C3—N2	−0.48 (17)	N1—C20—C25—C24	−174.72 (14)
C1—C2—C3—C4	178.03 (14)	C21—C20—C25—C24	1.5 (2)
N2—C3—C4—C5	2.5 (2)	C20—C21—C22—C23	−2.1 (3)
N2—C3—C4—C9	−178.89 (13)	C21—C22—C23—C24	1.8 (3)
C2—C3—C4—C5	−175.87 (15)	C22—C23—C24—C25	0.3 (3)
C2—C3—C4—C9	2.7 (2)	C23—C24—C25—C20	−1.8 (2)
C3—C4—C5—C6	178.05 (15)		