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Crystal structure and Hirshfeld surface analysis of 2,2′-(phenylazanediyl)bis(1-phenylethan-1-one)

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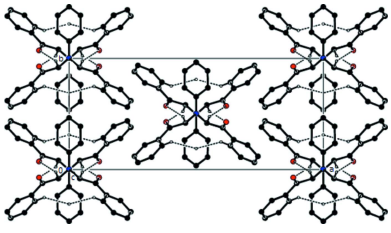
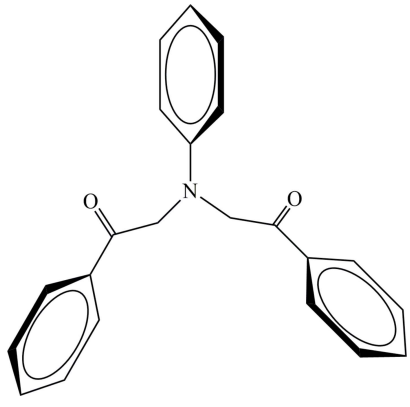
The whole molecule of the title compound, $C_{22}H_{19}NO_2$, is generated by twofold rotational symmetry. The N atom exhibits a trigonal-planar geometry and is located on the twofold rotation axis. In the crystal, molecules are linked by C—H···O contacts with $R_2^2(12)$ ring motifs, and C—H···π interactions, resulting in ribbons along the *c*-axis direction. van der Waals interactions between these ribbons consolidate the molecular packing. Hirshfeld surface analysis indicates that the greatest contributions to the crystal packing are from H···H (45.5%), C···H/H···C (38.2%) and O···H/H···O (16.0%) interactions.

1. Chemical context

Functionalized amine and carbonyl compounds are versatile intermediates in organic synthesis, material science and medicinal chemistry (Zubkov *et al.*, 2018; Shikhaliyev *et al.*, 2019; Viswanathan *et al.*, 2019; Gurbanov *et al.*, 2020). *N*,*N*-bis(phenacyl)anilines are of particular significance in the fine chemical industry due to their use as precursors of various heterocyclic systems such as piperidine, triazepine, 1,4-dihydropyrazine, 1,4-oxazine, pyrrole and indoles (Zeng & Chen, 2006; Ravindran *et al.*, 2007; Paul & Muthusubramanian, 2013; Yan *et al.*, 2014).





Thus, in the framework of our ongoing structural studies (Naghiyev *et al.*, 2020, 2021, 2022; Khalilov *et al.*, 2022), we report the crystal structure and Hirshfeld surface analysis of the title compound, 2,2′-(phenylazanediyl)bis(1-phenylethan-1-one).

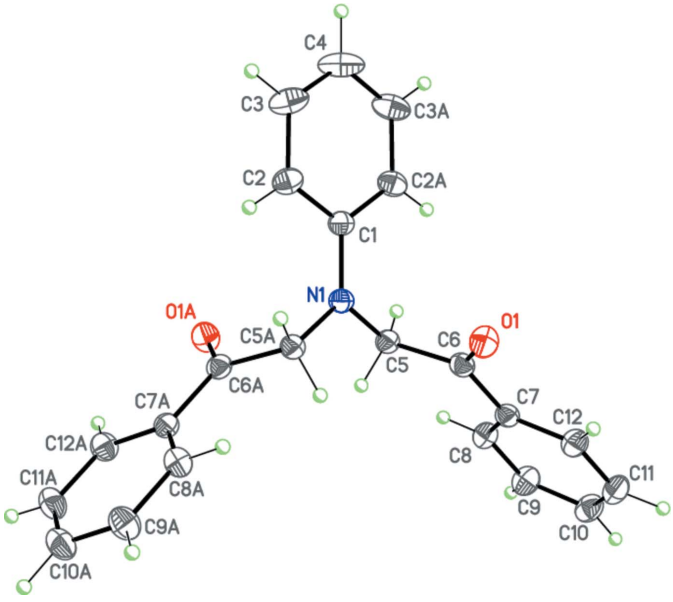


Figure 1
The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

2. Structural commentary

The asymmetric unit of the title compound contains half a molecule, the complete molecule being generated by the twofold rotational axis. Atoms N1, C1 and C4 are located on the twofold rotation axis (Fig. 1). The N1 atom has a trigonal-planar geometry, and it is bonded to two C atoms (C5 and C5*A*) from two symmetry-related 1-phenylethan-1-one groups and atom C1 of the phenyl ring, which is divided by the twofold rotation axis. The phenyl ring (C1–C4/C2*A*/C3*A*) attached to the N1 atom and the phenyl rings (C7–C12 and C7*A*–C12*A*) of the two symmetry-related 1-phenylethan-1-one groups are oriented at 89.65 (6)° to each other.

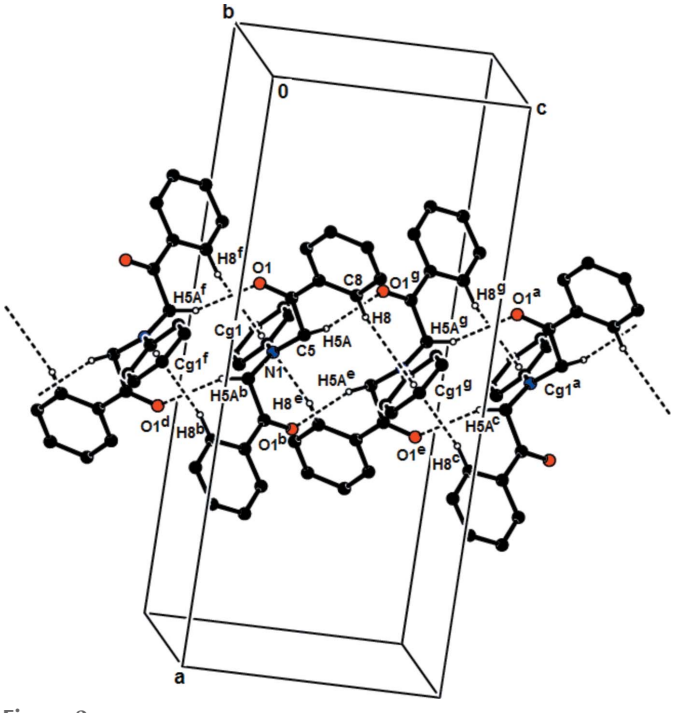


Figure 2
A general view of the intermolecular C—H···O hydrogen bonds, and C—H···π interactions of the title compound. The hydrogen atoms not involved in the hydrogen bonds have been omitted for clarity. Symmetry codes: (*a*) $x, y, z+1$; (*b*) $1-x, y, \frac{1}{2}-z$; (*c*) $x+\frac{3}{2}, -y+\frac{1}{2}, -z+1$; (*d*) $1-x, 1-y, -z$; (*e*) $1-x, 1-y, 1-z$; (*f*) $x, 1-y, -\frac{1}{2}+z$; (*g*) $x, 1-y, \frac{1}{2}+z$.

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

Cg1 is the centroid of the phenyl ring attached to atom N1.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5*A*···O1^{i}	0.99	2.51	3.4483 (16)	158
C8—H8···*Cg*1^{ii}	0.95	2.85	3.6963 (14)	148
C8—H8···*Cg*1^{iii}	0.95	2.85	3.6963 (14)	148

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

3. Supramolecular features and Hirshfeld surface analysis

In the crystal, molecules are linked by intermolecular C—H···O [C5—H5*A*···O1($x, -y+1, z+\frac{1}{2}$); 2.51 Å, 158°] interactions with $R_2^2(12)$ ring motifs, resulting in ribbons along the *c*-axis direction (Bernstein *et al.*, 1995; Table 1; Fig. 2). C—H···π interactions also contribute to the stronger cohesion of molecules in the ribbons (Table 1; Fig. 3). The molecular packing also features van der Waals interactions between these ribbons.

*Crystal Explorer*17.5 (Turner *et al.*, 2017) was used to perform a Hirshfeld surface analysis and generate the associated two-dimensional fingerprint plots, with a standard resolution of the three-dimensional d_{norm} surfaces plotted over a fixed colour scale of −0.1305 (red) to 1.2546 (blue) a.u (Fig. 4). In the Hirshfeld surface mapped over d_{norm} (Fig. 4), the bright-red spots near atoms O1 and H5*A* indicate the short C—H···O contacts (Table 1). Other contacts are equal to or longer than the sum of van der Waals radii.

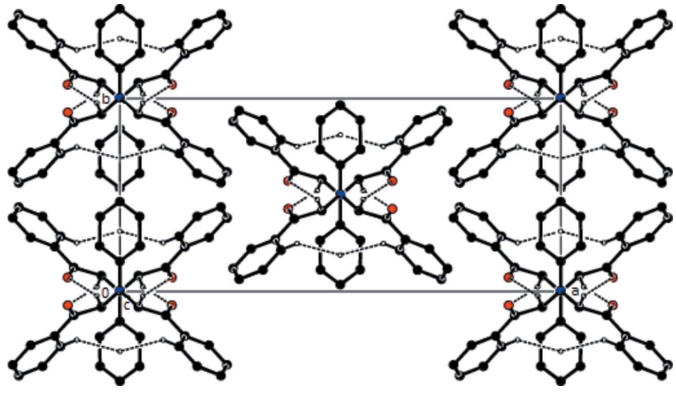


Figure 3
View of the packing down the *c* axis showing C—H···O hydrogen bonds and and C—H···π interactions in the title compound. The hydrogen atoms not involved in the hydrogen bonds have been omitted for clarity.

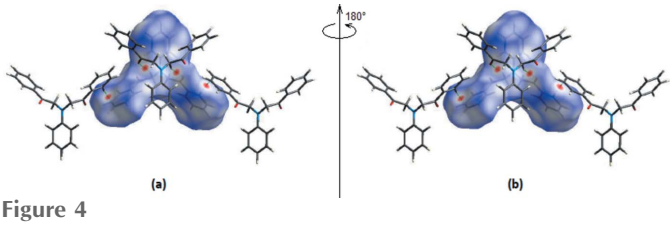


Figure 4
(*a*) Front and (*b*) back sides of the three-dimensional Hirshfeld surface of the title compound mapped over d_{norm}, with a fixed colour scale of −0.1305 to 1.2546 a.u. The C—H···O hydrogen bonds are shown.

Fingerprint plots (Fig. 5*b*–*d*; Table1) reveal that H···H (45.5%), C···H/H···C (38.2%) and O···H/H···O (16.0%) interactions make the greatest contributions to the surface contacts. N···H/H···N (0.3%) contacts also contribute to the overall crystal packing of the title compound. The Hirshfeld surface analysis confirms the importance of H-atom contacts in establishing the packing. The large number of H···H, C···H/H···C and O···H/H···O interactions suggest that van der Waals interactions and hydrogen bonding play the major roles in the crystal packing (Hathwar *et al.*, 2015).

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.42, update of September 2021; Groom *et al.*, 2016) for the *N*,*N*-dimethylaniline moiety revealed three structures closely related to the title compound, *viz*. 4-methyl-*N*-[(4-methylphenyl)sulfonyl]-*N*-phenylbenzenesulfonamide [CSD refcode GOBNIW (**I**); Eren *et al.*, 2014], *N*,*N*′-[(phenylimino)-diethane-2,1-diyl]bis(pyridine-2-carboxamide) [IDIZOM (**II**); Li *et al.*, 2013] and (2*E*,2′*E*)-dimethyl 2,2′-[(phenylazanediyl)bis(methylene)]bis(3-phenylacrylate) [XEBWUY (**III**); Sabari *et al.*, 2012]. Like the title compound, the molecule of (**I**) possesses twofold rotational symmetry. The N atom has a trigonal-planar geometry and is located on the twofold rotation axis. Weak C—H···O hydrogen bonds connect the molecules, forming a three-dimensional network. The asymmetric unit of (**II**) contains two independent molecules with similar conformations. In the crystal, N—H···O and weak C—H···O hydrogen bonds link the molecules into a three-dimensional supramolecular structure. Weak intermolecular C—H···π interactions are also observed. In (**III**), the C=C double bonds adopt an *E* configuration. In the crystal, pairs of C—H···O hydrogen bonds link the molecules into inversion dimers.

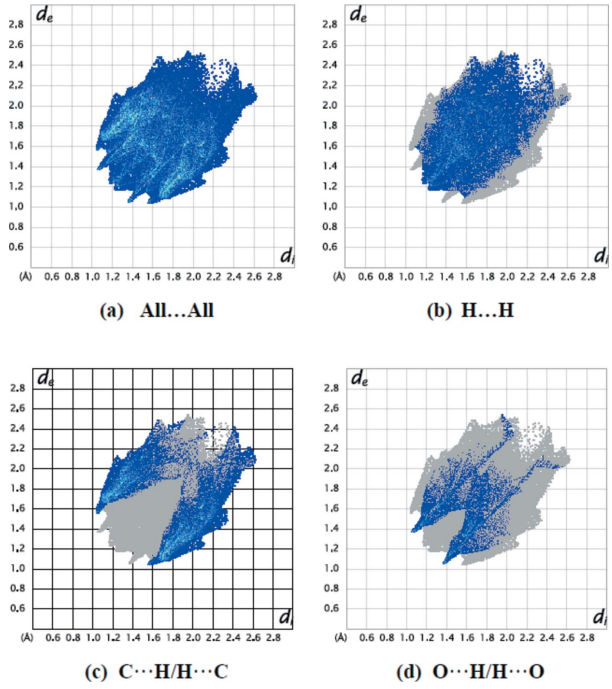


Figure 5
Two-dimensional fingerprint plots of the title compound, showing (*a*) all interactions, and delineated into (*b*) H···H, (*c*) C···H/H···C and (*d*) O···H/H···O interactions. [d_e and d_i represent the distances from a point on the Hirshfeld surface to the nearest atoms outside (external) and inside (internal) the surface, respectively].

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{22}H_{19}NO_2$
M_r	329.38
Crystal system, space group	Orthorhombic, *Pbcn*
Temperature (K)	100
a, *b*, *c* (Å)	20.8269 (2), 9.09843 (10), 9.0158 (1)
V (Å^3)	1708.42 (3)
Z	4
Radiation type	Cu *Kα*
μ (mm^{-1})	0.65
Crystal size (mm)	0.09 × 0.06 × 0.05
Data collection	
Diffractometer	XtaLAB Synergy, Dualflex, HyPix
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2021)
T_{min}, T_{max}	0.906, 0.939
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	21247, 1834, 1746
R_{int}	0.034
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.637
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.051, 0.142, 1.09
No. of reflections	1834
No. of parameters	115
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.29, −0.23

Computer programs: *CrysAlis PRO* (Rigaku OD, 2021), *SHELXT2014/5* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2020).

5. Synthesis and crystallization

The title compound was synthesized using the reported procedure (He *et al.*, 2014), and pale-yellow needle-like crystals were obtained upon slow evaporation from an ethanol/water (4:1) homogeneous solution at room temperature.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms bound to C atoms

were positioned geometrically (C—H = 0.95 and 0.99 Å) and refined using a riding model with U_{iso}(H) = 1.2U_{eq}(C). Owing to poor agreement between observed and calculated intensities, eighteen outliers (8 1 3, 1 5 6, 25 0 2, 4 5 3, 2 7 3, 1 2 3, 1 1 6, 7 3 0, 14 3 9, 5 3 0, 4 5 8, 0 4 0, 21 0 2, 7 4 8, 9 10 3, 2 4 0, 23 2 2, 2 8 5) were omitted during the final refinement cycle.

Acknowledgements

Authors' contributions are as follows. Conceptualization, ANK and IGM; methodology, ANK and IGM; investigation, ANK, MA and MGS; writing (original draft), MA and ANK; writing (review and editing of the manuscript), MA and ANK; visualization, MA, ANK and IGM; funding acquisition, VNK, FNN and ANK; resources, AB, VNK and FNN; supervision, ANK and MA.

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References

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.

Eren, B., Demir, S., Dal, H. & Hökelek, T. (2014). *Acta Cryst.* E**70**, o238–o239.

Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.

Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.

Gurbanov, A. V., Kuznetsov, M. L., Demukhamedova, S. D., Alieva, I. N., Godjaev, N. M., Zubkov, F. I., Mahmudov, K. T. & Pombeiro, A. J. L. (2020). *CrystEngComm*, **22**, 628–633.

Hathwar, V. R., Sist, M., Jørgensen, M. R. V., Mamakhel, A. H., Wang, X., Hoffmann, C. M., Sugimoto, K., Overgaard, J. & Iversen, B. B. (2015). *IUCrJ*, **2**, 563–574.

He, J., Shi, L., Liu, S., Jia, P., Wang, J. & Hu, R. (2014). *Monatsh. Chem.* **145**, 213–216.

Khalilov, A. N., Khrustalev, V. N., Tereshina, T. A., Akkurt, M., Rzayev, R. M., Akobirshoeva, A. A. & Mamedov, İ. G. (2022). *Acta Cryst.* E**78**, 525–529.

Li, G.-N., Niu, Z.-G., Huang, M.-Q., Zou, Y. & Hu, L.-J. (2013). *Acta Cryst.* E**69**, o677.

Naghiyev, F. N., Akkurt, M., Askerov, R. K., Mamedov, I. G., Rzayev, R. M., Chyrka, T. & Maharramov, A. M. (2020). *Acta Cryst.* E**76**, 720–723.

Naghiyev, F. N., Khrustalev, V. N., Novikov, A. P., Akkurt, M., Rzayev, R. M., Akobirshoeva, A. A. & Mamedov, I. G. (2022). *Acta Cryst.* E**78**, 554–558.

Naghiyev, F. N., Tereshina, T. A., Khrustalev, V. N., Akkurt, M., Rzayev, R. M., Akobirshoeva, A. A. & Mamedov, İ. G. (2021). *Acta Cryst.* E**77**, 516–521.

Paul, N. & Muthusubramanian, S. (2013). *Synth. Commun.* **43**, 1200–1209.

Ravindran, G., Muthusubramanian, S., Selvaraj, S. & Perumal, S. (2007). *J. Heterocycl. Chem.* **44**, 133–136.

Rigaku OD (2021). *CrysAlis PRO*. Rigaku Oxford Diffraction, Yarnton, England.

Sabari, V., Selvakumar, R., Bakthadoss, M. & Aravindhan, S. (2012). *Acta Cryst.* E**68**, o2265.

Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

Shikhaliyev, N. Q., Kuznetsov, M. L., Maharramov, A. M., Gurbanov, A. V., Ahmadova, N. E., Nenajdenko, V. G., Mahmudov, K. T. & Pombeiro, A. J. L. (2019). *CrystEngComm*, **21**, 5032–5038.

Spek, A. L. (2020). *Acta Cryst.* E**76**, 1–11.

Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Spackman, P. R., Jayatilaka, D. & Spackman, M. A. (2017). *CrystalExplorer17. University of Western Australia.* http://Hirshfeldsurface.net.

Viswanathan, A., Kute, D., Musa, A., Konda Mani, S., Sipilä, V., Emmert-Streib, F., Zubkov, F. I., Gurbanov, A. V., Yli-Harja, O. & Kandhavelu, M. (2019). *Eur. J. Med. Chem.* **166**, 291–303.

Yan, H., Tan, H. & Xin, H. (2014). *Heterocycles*, **89**, 359–373.

Zeng, D. X. & Chen, Y. (2006). *Synlett*, pp. 0490–0492.

Zubkov, F. I., Mertsalov, D. F., Zaytsev, V. P., Varlamov, A. V., Gurbanov, A. V., Dorovatovskii, P. V., Timofeeva, T. V., Khrustalev, V. N. & Mahmudov, K. T. (2018). *J. Mol. Liq.* **249**, 949–952.

supporting information

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Farid N. Naghiyev, Victor N. Khrustalev, Marina G. Safronenko, Mehmet Akkurt, Ali N. Khalilov, Ajaya Bhattarai and İbrahim G. Mamedov

Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2021); cell refinement: *CrysAlis PRO* (Rigaku OD, 2021); data reduction: *CrysAlis PRO* (Rigaku OD, 2021); program(s) used to solve structure: *SHELXT2014/5* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015b); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2020).

2,2′-(Phenylazanediyl)bis(1-phenylethan-1-one)

Crystal data

$C_{22}H_{19}NO_2$
$M_r = 329.38$
Orthorhombic, *Pbcn*
$a = 20.8269$ (2) Å
$b = 9.09843$ (10) Å
$c = 9.0158$ (1) Å
$V = 1708.42$ (3) Å^3
$Z = 4$
$F(000) = 696$
$D_x = 1.281$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 14002 reflections
$\theta = 4.3$–$79.0°$
$\mu = 0.65$ mm^{-1}
$T = 100$ K
Prism, pale yellow
0.09 × 0.06 × 0.05 mm

Data collection

XtaLAB Synergy, Dualflex, HyPix diffractometer
Radiation source: micro-focus sealed X-ray tube
φ and ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2021)
$T_{min} = 0.906$, $T_{max} = 0.939$
21247 measured reflections
1834 independent reflections
1746 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 79.4°$, $\theta_{min} = 4.3°$
$h = -26\rightarrow26$
$k = -11\rightarrow10$
$l = -10\rightarrow11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.142$
$S = 1.09$
1834 reflections
115 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0811P)^2 + 0.6375P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

Special details

Experimental. CrysAlisPro 1.171.41.117a (Rigaku OD, 2021) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.38204 (5)	0.42787 (12)	0.14622 (11)	0.0346 (3)
N1	0.500000	0.50356 (17)	0.250000	0.0275 (4)
C1	0.500000	0.65552 (19)	0.250000	0.0258 (4)
C2	0.54585 (7)	0.73540 (15)	0.16825 (14)	0.0312 (3)
H2	0.577660	0.684521	0.112882	0.037*
C3	0.54488 (9)	0.88824 (18)	0.16798 (17)	0.0432 (4)
H3	0.575533	0.940593	0.110555	0.052*
C4	0.500000	0.9651 (2)	0.250000	0.0537 (7)
H4	0.499999	1.069489	0.250000	0.064*
C5	0.45804 (6)	0.41853 (14)	0.34384 (14)	0.0256 (3)
H5A	0.447899	0.476190	0.433961	0.031*
H5B	0.480651	0.328071	0.375413	0.031*
C6	0.39556 (6)	0.37610 (14)	0.26663 (14)	0.0262 (3)
C7	0.35248 (6)	0.26878 (14)	0.34230 (13)	0.0256 (3)
C8	0.36541 (6)	0.21454 (15)	0.48403 (15)	0.0304 (3)
H8	0.402012	0.248116	0.537005	0.036*
C9	0.32461 (7)	0.11135 (17)	0.54737 (16)	0.0362 (4)
H9	0.333629	0.073789	0.643461	0.043*
C10	0.27080 (7)	0.06284 (17)	0.47116 (17)	0.0362 (4)
H10	0.243425	−0.008843	0.514406	0.043*
C11	0.25697 (7)	0.11905 (17)	0.33172 (16)	0.0353 (4)
H11	0.219476	0.087802	0.280639	0.042*
C12	0.29775 (7)	0.22064 (15)	0.26696 (16)	0.0316 (3)
H12	0.288486	0.257788	0.170838	0.038*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0336 (5)	0.0400 (6)	0.0302 (5)	−0.0032 (4)	−0.0024 (4)	0.0071 (4)
N1	0.0260 (7)	0.0226 (7)	0.0338 (8)	0.000	0.0068 (6)	0.000
C1	0.0285 (8)	0.0239 (8)	0.0250 (8)	0.000	−0.0043 (6)	0.000
C2	0.0378 (8)	0.0281 (7)	0.0277 (7)	−0.0037 (5)	−0.0006 (5)	0.0014 (5)
C3	0.0632 (11)	0.0286 (7)	0.0378 (8)	−0.0102 (7)	0.0028 (7)	0.0047 (6)
C4	0.091 (2)	0.0228 (10)	0.0475 (13)	0.000	0.0033 (12)	0.000
C5	0.0251 (6)	0.0241 (6)	0.0277 (6)	−0.0004 (4)	0.0020 (4)	0.0007 (4)
C6	0.0266 (6)	0.0247 (6)	0.0272 (6)	0.0028 (5)	0.0027 (5)	−0.0019 (5)
C7	0.0254 (6)	0.0236 (6)	0.0277 (6)	0.0014 (5)	0.0035 (4)	−0.0028 (4)

C8	0.0292 (6)	0.0326 (7)	0.0292 (6)	−0.0036 (5)	0.0009 (5)	−0.0009 (5)
C9	0.0377 (7)	0.0407 (8)	0.0303 (7)	−0.0064 (6)	0.0040 (6)	0.0041 (6)
C10	0.0352 (7)	0.0367 (7)	0.0366 (7)	−0.0092 (6)	0.0086 (6)	−0.0019 (6)
C11	0.0305 (7)	0.0382 (8)	0.0372 (8)	−0.0086 (6)	0.0014 (5)	−0.0063 (6)
C12	0.0316 (7)	0.0328 (7)	0.0304 (7)	−0.0024 (5)	−0.0009 (5)	−0.0019 (5)

Geometric parameters (Å, º)

O1—C6	1.2165 (16)	C5—H5B	0.9900
N1—C1	1.383 (2)	C6—C7	1.4913 (18)
N1—C5	1.4415 (14)	C7—C8	1.3960 (19)
N1—C5^{i}	1.4416 (14)	C7—C12	1.3973 (19)
C1—C2^{i}	1.4082 (16)	C8—C9	1.3892 (19)
C1—C2	1.4082 (16)	C8—H8	0.9500
C2—C3	1.391 (2)	C9—C10	1.387 (2)
C2—H2	0.9500	C9—H9	0.9500
C3—C4	1.382 (2)	C10—C11	1.388 (2)
C3—H3	0.9500	C10—H10	0.9500
C4—H4	0.9500	C11—C12	1.384 (2)
C5—C6	1.5254 (17)	C11—H11	0.9500
C5—H5A	0.9900	C12—H12	0.9500
C1—N1—C5	122.46 (7)	O1—C6—C7	121.50 (12)
C1—N1—C5^{i}	122.46 (7)	O1—C6—C5	120.45 (11)
C5—N1—C5^{i}	115.08 (14)	C7—C6—C5	118.05 (11)
N1—C1—C2^{i}	121.07 (9)	C8—C7—C12	119.44 (12)
N1—C1—C2	121.07 (9)	C8—C7—C6	122.28 (12)
C2^{i}—C1—C2	117.86 (17)	C12—C7—C6	118.27 (12)
C3—C2—C1	120.47 (14)	C9—C8—C7	119.81 (13)
C3—C2—H2	119.8	C9—C8—H8	120.1
C1—C2—H2	119.8	C7—C8—H8	120.1
C4—C3—C2	120.98 (15)	C10—C9—C8	120.38 (13)
C4—C3—H3	119.5	C10—C9—H9	119.8
C2—C3—H3	119.5	C8—C9—H9	119.8
C3^{i}—C4—C3	119.2 (2)	C9—C10—C11	119.97 (13)
C3^{i}—C4—H4	120.4	C9—C10—H10	120.0
C3—C4—H4	120.4	C11—C10—H10	120.0
N1—C5—C6	112.65 (9)	C12—C11—C10	120.05 (13)
N1—C5—H5A	109.1	C12—C11—H11	120.0
C6—C5—H5A	109.1	C10—C11—H11	120.0
N1—C5—H5B	109.1	C11—C12—C7	120.32 (13)
C6—C5—H5B	109.1	C11—C12—H12	119.8
H5A—C5—H5B	107.8	C7—C12—H12	119.8
C5—N1—C1—C2^{i}	−6.40 (9)	O1—C6—C7—C8	−176.33 (12)
C5^{i}—N1—C1—C2^{i}	173.60 (9)	C5—C6—C7—C8	4.37 (18)
C5—N1—C1—C2	173.59 (9)	O1—C6—C7—C12	4.30 (19)
C5^{i}—N1—C1—C2	−6.41 (9)	C5—C6—C7—C12	−175.00 (11)

N1—C1—C2—C3	179.32 (10)	C12—C7—C8—C9	1.3 (2)
C2^{i}—C1—C2—C3	−0.68 (10)	C6—C7—C8—C9	−178.06 (12)
C1—C2—C3—C4	1.4 (2)	C7—C8—C9—C10	−0.6 (2)
C2—C3—C4—C3^{i}	−0.69 (11)	C8—C9—C10—C11	−0.9 (2)
C1—N1—C5—C6	93.41 (9)	C9—C10—C11—C12	1.7 (2)
C5^{i}—N1—C5—C6	−86.59 (9)	C10—C11—C12—C7	−1.0 (2)
N1—C5—C6—O1	−8.70 (17)	C8—C7—C12—C11	−0.6 (2)
N1—C5—C6—C7	170.61 (11)	C6—C7—C12—C11	178.84 (12)

Symmetry code: (i) −*x*+1, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the phenyl ring attached to atom N1.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5*A*···O1^{ii}	0.99	2.51	3.4483 (16)	158
C8—H8···*Cg*1^{iii}	0.95	2.85	3.6963 (14)	148
C8—H8···*Cg*1^{iv}	0.95	2.85	3.6963 (14)	148

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