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

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

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).
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 C5A) 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/C2A/C3A) attached to the N1 atom and the phenyl rings (C7–C12 and C7A–C12A) of the two symmetry-related 1-phenylethan-1-one groups are oriented at 89.65 (6)° to each other.

3. Supramolecular features and Hirshfeld surface analysis

In the crystal, molecules are linked by intermolecular C—H···O [C5—H5A···O1i 0.99 2.51 3.4483 (16) 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 Explorer17.5 (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 H5A 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 1](image1.png)

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

![Figure 2](image2.png)

**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, 1/2 − z; (c) x + 1/2, −y + 1/2, −z + 1; (d) 1 − x, 1 − y, −z; (e) 1 − x, 1 − y, 1 − z; (f) x, 1 − y, −1/2 + z; (g) x, 1 − y, 1/2 + z.

![Figure 3](image3.png)

**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.

| D—H···A | D—H | H···A | D···A | D—H···A |
|---------|------|-------|-------|---------|
| C5—H5A···O1i | 0.99 | 2.51 | 3.4483 (16) | 158 |
| C8—HB···Cg1iv | 0.95 | 2.85 | 3.6963 (14) | 148 |

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

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

\( Cg1 \) is the centroid of the phenyl ring attached to atom N1.
Fingerprint plots (Fig. 5b–d; Table 1) 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 inside (internal) and outside (external) the surface, respectively.

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 (2E,2’E)-dimethyl 2,2’-[phenylazanediyl]bis(methylene)bis(3-phenylacylate) [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.

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 treated as riding with C–H bond lengths of 0.93 Å.

Table 2
Experimental details.

| Crystal data | Chemical formula | C22H19NO2 |
|--------------|------------------|------------|
| Chemical formula | M<sub>r</sub> | 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 (Å³) | 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 | XtaLAB Synergy, Dualflex, HyPix Multi-scan (CrysAlis PRO; Rigaku OD, 2021) |
| Absorption correction | CrysAlis PRO (Spek, 2020) |
| No. of measured, independent and observed [I > 2σ(I)] reflections | 21247, 1834, 1746 |
| R<sub>int</sub>, wR<sub>2</sub>, S | 0.051, 0.142, 1.09 |
| No. of reflections | 1834 |
| No. of parameters | 115 |
| H-atom treatment | H-atom parameters constrained |
| Δρ<sub>max</sub>, Δρ<sub>min</sub> (e Å⁻³) | 0.29, −0.23 |

Computer programs: CrysAlis PRO (Rigaku OD, 2021), SHELXT2014/5 (Sheldrick, 2013a), SHELXL2018/3 (Sheldrick, 2015b), ORTEP-3 for Windows (Farrugia, 2012) and PLATON (Spek, 2020).
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, 2 5 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, 2 1 0 2, 7 4 8, 9 1 0 3, 2 4 0, 23 2 2, 2 8 5) were omitted during the final refinement cycle.

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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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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

C22H19NO2  
Mr = 329.38  
Orthorhombic, Pbcn  
a = 20.8269 (2) Å  
b = 9.09843 (10) Å  
c = 9.0158 (1) Å  
V = 1708.42 (3) Å3  
Z = 4  
F(000) = 696

Data collection

XtaLAB Synergy, Dualflex, HyPix diffractometer  
Radiation source: micro-focus sealed X-ray tube  
φ and ω scans  
(CrysAlisPro; Rigaku OD, 2021)  
Tmin = 0.906, Tmax = 0.939  
21247 measured reflections

Refinement

Refinement on F2  
Least-squares matrix: full  
R[F2 > 2σ(F2)] = 0.051  
wR(F2) = 0.142  
S = 1.09  
1834 reflections  
115 parameters  
0 restraints

Hydrogen site location: inferred from neighbouring sites  
H-atom parameters constrained  
\[ w = \frac{1}{\sigma^2(F_o^2) + (0.0811P)^2 + 0.6375P} \]  
where P = (Fo^2 + 2Fc^2)/3  
(Δ/σ)max < 0.001  
Δρmax = 0.28 e Å⁻³  
Δρmin = -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     | Uiso* / Ueq |
|---|-------|-------|-------|-------------|
| 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 | 0.68452 | 0.11288 | 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)

|   | U11 | U22 | U33 | U12 | U13 | U23 |
|---|-----|-----|-----|-----|-----|-----|
| 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) |


| Atomic Number | U11 (Å²) | U22 (Å²) | U33 (Å²) | U12 (Å²) | U13 (Å²) | U23 (Å²) |
|---------------|----------|----------|----------|----------|----------|----------|
| C8            | 0.0292   | 0.0326   | 0.0292   | −0.0036  | 0.0009   | −0.0009  |
| C9            | 0.0377   | 0.0407   | 0.0303   | −0.0064  | 0.0040   | 0.0041   |
| C10           | 0.0352   | 0.0367   | 0.0366   | −0.0092  | 0.0086   |−0.0019   |
| C11           | 0.0305   | 0.0382   | 0.0372   | −0.0086  | 0.0014   |−0.0063   |
| C12           | 0.0316   | 0.0328   | 0.0304   | −0.0024  | −0.0009  |−0.0019   |

| Geometric parameters (Å, °) |
|-----------------------------|
| 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—C5i 1.4416 (14) C7—C12 1.3973 (19) |
| C1—C2i 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—C5i 122.46 (7) O1—C6—C5 120.45 (11) |
| C5—N1—C5i 115.08 (14) C7—C6—C5 118.05 (11) |
| N1—C1—C2i 121.07 (9) C8—C7—C12 119.44 (12) |
| N1—C1—C2 121.07 (9) C8—C7—C6 122.28 (12) |
| C2—C1—C2 117.86 (17) C12—C7—C6 118.27 (12) |
| C2—C3—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—C4—C3 119.2 (2) C9—C10—C11 119.97 (13) |
| C3—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—C2i −6.40 (9) O1—C6—C7—C8 −176.33 (12) |
| C5—N1—C1—C2 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—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)
C2i—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—C3i −0.69 (11) C8—C9—C10—C11 −0.9 (2)
C1—N1—C5—C6 93.41 (9) C9—C10—C11—C12 1.7 (2)
C5i—N1—C5—C6 −86.59 (9) C10—C11—C12—C7 −1.0 (2)
N1—C5—C6—O1 −8.70 (17) C11—C12—C7—C12 −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, °)

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—H5A···O1ii | 0.99 | 2.51 | 3.4483 (16) | 158 |
| C8—H8···Cg1iii | 0.95 | 2.85 | 3.6963 (14) | 148 |
| C8—H8···Cg1iv | 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.