



Received 10 October 2017

Accepted 11 October 2017

Edited by P. C. Healy, Griffith University,
Australia‡ Additional correspondence author, e-mail:
edwardt@sunway.edu.my.**Keywords:** crystal structure; 1,2,3-triazole;
Hirshfeld surface analysis.**CCDC reference:** 1579464**Supporting information:** this article has
supporting information at journals.iucr.org/e

4-Benzyl-1-(4-nitrophenyl)-1*H*-1,2,3-triazole: crystal structure and Hirshfeld analysis

Julio Zukerman-Schpector,^{a*} Sofia Dallasta Pedroso,^a Lucas Sousa Madureira,^a
Márcio Weber Paixão,^b Akbar Ali^b and Edward R. T. Tiekink^{c‡}^aLaboratório de Cristalografia, Esterodinâmica e, Modelagem Molecular, Departamento de Química, Universidade Federal de São Carlos, 13565-905 São Carlos, SP, Brazil, ^bDepartamento de Química, Universidade Federal de São Carlos, 13565-905 São Carlos, SP, Brazil, and ^cResearch Centre for Crystalline Materials, School of Science and Technology, Sunway University, 47500 Bandar Sunway, Selangor Darul Ehsan, Malaysia. *Correspondence e-mail: julio@power.ufscar.br

The molecule in the title compound, C₁₅H₁₂N₄O₂, has a twisted *L*-shape with the dihedral angle between the aromatic rings of the N-bound benzene and C-bound benzyl groups being 70.60 (9)°. The nitro group is co-planar with the benzene ring to which it is connected [C–C–N–O torsion angle = 0.4 (3)°]. The three-dimensional packing is stabilized by a combination of methylene–C–H···O(nitro), methylene–C–H···π(phenyl), phenyl–C–H···π(triazolyl) and nitro–O···π(nitrobenzene) interactions, along with weak π(triazolyl)–π(nitrobenzene) contacts [inter-centroid distance = 3.8386 (10) Å]. The importance of the specified intermolecular contacts has been verified by an analysis of the calculated Hirshfeld surface.

1. Chemical context

The 1,2,3-triazoles comprise an important class of molecules, having a number of applications in biology and materials science. As reviewed recently, 1,2,3-triazoles display various potential pharmaceutical properties including anti-cancer, anti-viral, anti-tuberculosis and anti-microbial activities (Tron *et al.*, 2008; Thirumurugan *et al.*, 2013). The 1,2,3-triazole chromophore can function as a most useful scaffold in bio-conjugation owing to its rigid framework, stability, and, crucially, water-solubility (Jewett & Bertozzi, 2010; Holub & Kirshenbaum, 2010). Further applications are known in the fields of dyes, photostabilizers and as agrochemicals (Golas & Matyjaszewski, 2010; Qin *et al.*, 2010). Very recently, a new and efficient synthesis for a metal-free and regioselective synthesis of 1,4-disubstituted 1,2,3-triazoles was described (Ali *et al.*, 2014). Among the compounds synthesized in that study was the title compound, (I). Herein, the crystal and molecular structures of (I) are described along with an analysis of the Hirshfeld surface.

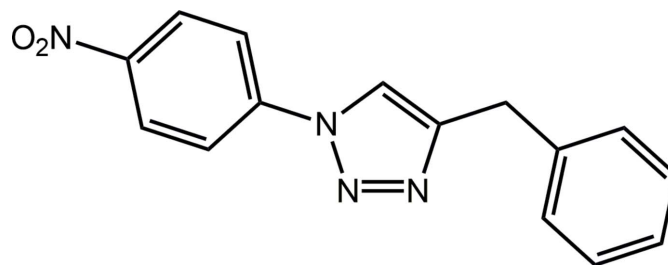
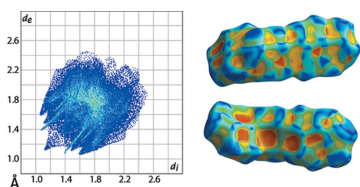


Table 1

Hydrogen-bond geometry (Å, °).

Cg1–Cg3 are the centroids of the N1–N3, C1, C2, C4–C9 and C10–C15 rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C3–H3B \cdots O2 ⁱ	0.97	2.58	3.452 (3)	150
C3–H3A \cdots Cg2 ⁱⁱ	0.97	2.96	3.857 (2)	154
C8–H8 \cdots Cg1 ⁱⁱⁱ	0.93	2.86	3.665 (3)	146
N4–O1 \cdots Cg3 ^{iv}	1.21 (1)	3.67 (1)	4.1254 (19)	103 (1)

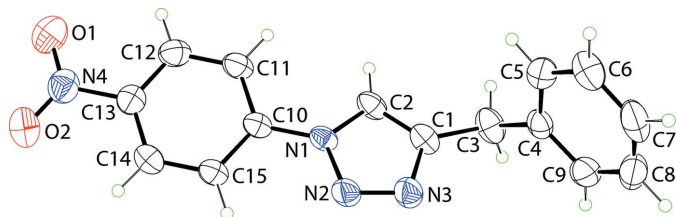
 Symmetry codes: (i) $-x+1, -y, -z+2$; (ii) $x-1, y, z$; (iii) $-x+2, y-\frac{1}{2}, -z+\frac{3}{2}$; (iv) $-x+1, -y+1, -z+2$.

2. Structural commentary

The molecular structure of (I), Fig. 1, comprises a central, strictly planar 1,2,3-triazolyl ring (r.m.s. deviation of the five fitted atoms = 0.001 Å) flanked by C- and N-bound benzyl and 4-nitrobenzene substituents, respectively. The dihedral angle between the five-membered ring and phenyl ring is 83.23 (10)°, indicating a near perpendicular relationship. By contrast, the benzene ring is closer to co-planar to the triazolyl ring, forming a dihedral angle of 13.95 (9)°. The dihedral angle between the outer rings is 70.60 (9)°, indicating that the molecule has a skewed-shape based on the letter *L*. The nitro group is co-planar with the benzene ring to which it is bound as seen in the value of the C12–C13–N4–O1 torsion angle of 0.4 (3)°.

3. Supramolecular features

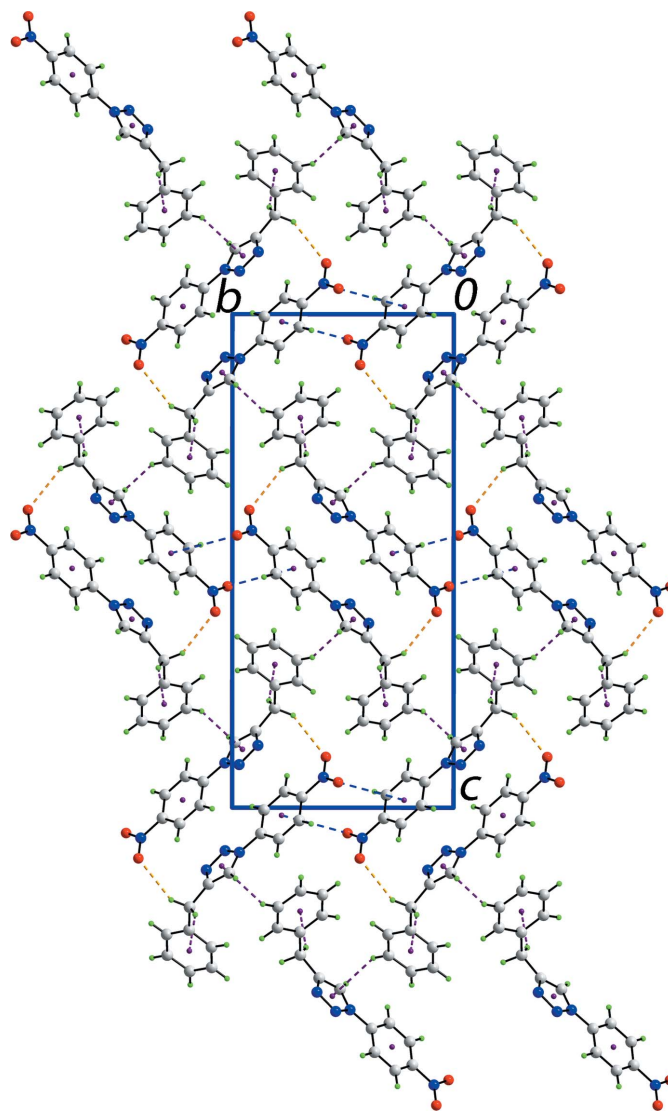
The molecular packing of (I) features methylene-C–H \cdots O(nitro), methylene-C–H \cdots π (phenyl), phenyl-C–H \cdots π (triazolyl) and nitro-O \cdots π (nitrobenzene) interactions, Table 1; the latter interactions have been described as being important in stabilizing the crystal packing of nitro-containing compounds (Huang *et al.*, 2008). The C–H \cdots O and nitro-O \cdots π interactions occur between centrosymmetrically related molecules while the C–H \cdots π (phenyl) contacts occur along the *a*-axis direction and the C–H \cdots π (triazolyl) contacts along the *b*-axis direction and, all taken together, consolidate the three-dimensional architecture, Fig. 2. Within the specified framework, weak π (triazolyl) \cdots π (nitrobenzene)ⁱ interactions occur with the inter-centroid distance = 3.8386 (10) Å, interplanar angle = 13.95 (9)° for symmetry code: (i) $1-x, -y, 2-z$.


Figure 1

The molecular structure of (I), showing the atom-labelling scheme and displacement ellipsoids at the 35% probability level.

4. Hirshfeld surface analysis

The study of the Hirshfeld surface and intermolecular interactions of (I) has been carried out using standard parameters of the *CrystalExplorer* package (Wolff *et al.*, 2012) and using similar protocols as in earlier studies (Zukerman-Schpector *et al.*, 2017). In (I), the Hirshfeld surface is controlled by attractive interactions such as non-conventional C–H \cdots π , C–H \cdots O, C–H \cdots N hydrogen bonds and π – π interactions. The aforementioned contacts contribute around 70% to the overall surface area, Fig. 3 and Table 2. The repulsive H \cdots H interactions account for the remaining 30%, Fig. 3b. These observations may be rationalized in terms of the structure having electron-rich groups, *i.e.* the three aromatic rings and the nitro substituent, for which the electron densities are highly delocalized allowing them to have significant overlap in the molecular packing.


Figure 2

A view of the unit-cell contents in projection down the *a* axis. The C–H \cdots O, C–H \cdots π and nitro-O \cdots π contacts are shown as orange, purple and blue dashed lines, respectively.

Table 2
Percentage contributions of interatomic contacts to the Hirshfeld surface for (I).

Contact	Percentage contribution
H···H	28.7
C···H/H···C	26.1
O···H/H···O	21.0
N···H/H···N	15.6
C···N/N···C	3.9
C···O/O···C	2.4
others	2.3

Table 3
Summary of short interatomic contacts (Å) in (I).

Contact	Distance	Symmetry operation
H15···H15	2.54	$2 - x, -y, 2 - z$
C7···H11	2.78	$1 - x, -\frac{1}{2} + y, \frac{3}{2} - z$
O1···H12	2.62	$-x, 1 - y, 2 - z$
O1···C13	3.386 (3)	$1 - x, 1 - y, 2 - z$
C15···N1	3.413 (2)	$1 - x, -y, 2 - z$
H15···N2	2.71	$2 - x, -y, 2 - z$
H14···N3	3.00	$2 - x, -y, 2 - z$

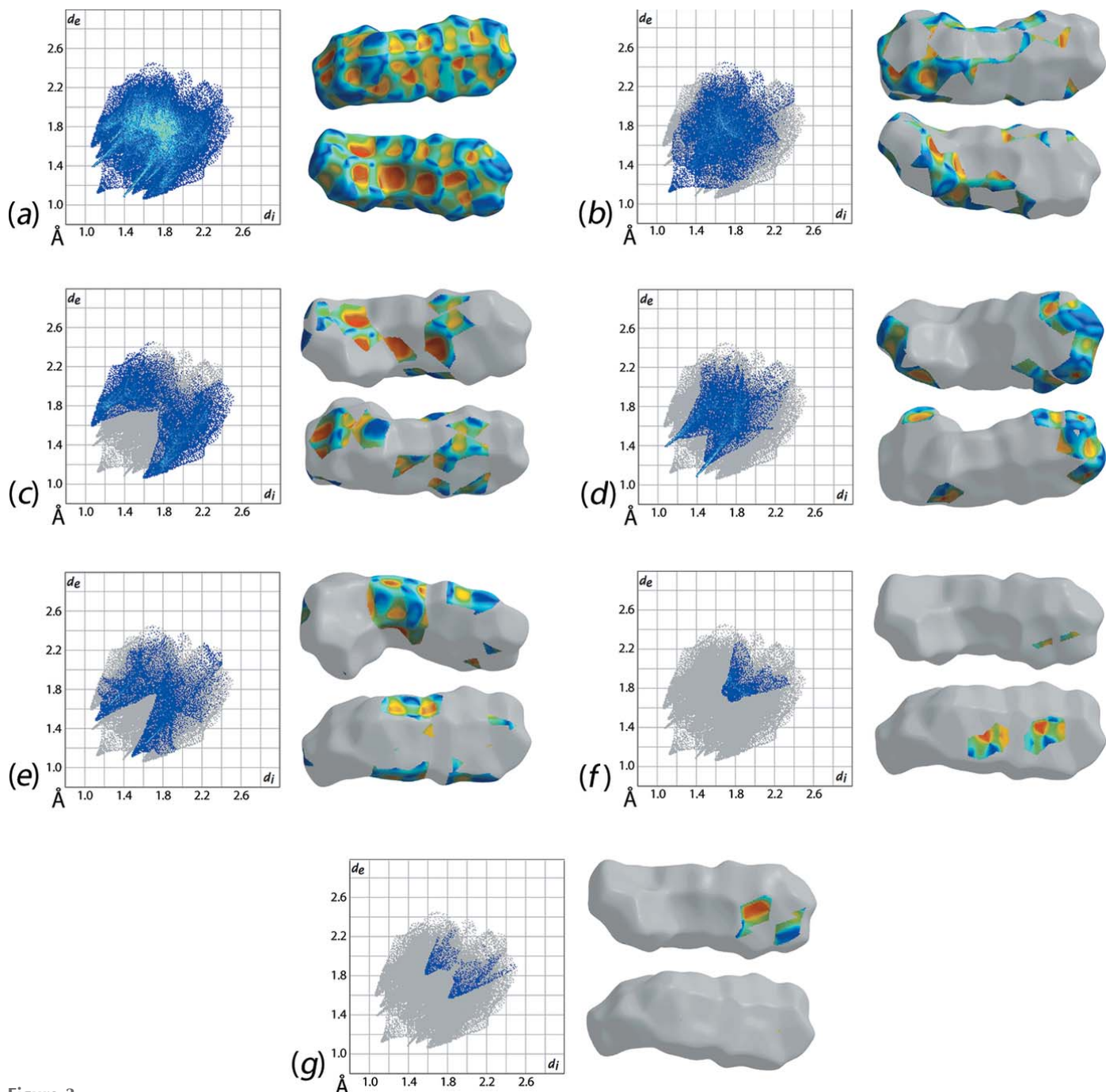


Figure 3
(a) The full two-dimensional fingerprint plot for (I) and two views of the Hirshfeld surface mapped over the shape-index property, and fingerprint plots delineated into (b) H···H, (c) C···H/H···C, (d) O···H/H···O, (e) N···H/H···N, (f) C···N/N···C and (g) C···O/O···C interatomic contacts along with two views of Hirshfeld surface mapped over shape-index.

As attractive interactions, the C··H/H··C contacts contribute a significant role (26.1%) to the overall surface area. These contacts arise mainly from C—H·· π contacts spread over the entire molecule in which all rings, *i.e.* the triazole, nitrobenzene and benzyl rings, function as H-atom acceptors, Tables 1 and 3, and Fig. 3c. The O··H/H··O contacts contribute 21.0% to the Hirshfeld surface area. In essence, this arises owing to non-conventional C—H··O hydrogen bonds, Fig. 3d. There are two different H-donor carbon atoms participating in the weak C—H··O interactions, one of which is the methylene-C3 atom, Table 1, and the other being the nitrobenzene-C12 atom, Table 3. The N··H/H··N contacts contribute approximately 16% to the overall surface area, Fig. 3e. Non conventional C—H··N hydrogen bonds are formed with nitrobenzene-C atoms as H-atom donors, Table 3 and Fig. 3f. The C··N/N··C and C··O/O··C contacts contribute around 6% to the Hirshfeld surface, Table 2 and Fig. 3f and g. Other surface contacts do not contribute significantly to the molecular packing.

5. Database survey

There are only relatively few 1,2,3-triazole structures in the literature having N-bound aryl groups and C-bound alkyl substituents. The two molecules closest to (I) have N-bound 4-chlorobenzene and C-bound *n*-butyl groups, *i.e.* (II) (Sarode *et al.*, 2016), and N-bound 4-nitrobenzene and C-bound *n*-hexyl groups, *i.e.* (III) (Muhammad *et al.*, 2015). In (II), the dihedral angle between the two planes is 22.59 (7)° and the *n*-butyl group is co-planar with the the five-membered ring as seen in the $sp^2\text{-C}-\text{C}_{\text{quaternary}}-\text{C}-\text{C}_{\text{methylene}} = 0.06$ (4)° and $\text{C}_{\text{methylene}}-\text{C}-\text{C}-\text{C}_{\text{methyl}} = -177.39$ (19)° torsion angles. In (III), the aromatic rings are considerably more co-planar, *cf.* (I) and (II), with the dihedral angle between them being 2.65 (8)°. With respect to the *n*-hexyl substituent, the structure of (III) resembles that of (I) in that the $sp^2\text{-C}-\text{C}_{\text{quaternary}}-\text{C}-\text{C}_{\text{methylene}}$ torsion angle is -118.4 (3)°.

6. Synthesis and crystallization

The title compound was prepared as described in the literature (Ali *et al.*, 2014). Crystals of (I) for the X-ray study were obtained by slow evaporation from an ethyl acetate/*n*-hexane solution (5:1 *v/v*). ¹H NMR (400 MHz, CDCl₃) δ 7.70–7.65 (*m*, 2H), 7.59 (*s*, 1H), 7.51–7.45 (*m*, 2H), 7.42–7.32 (*m*, 3H), 7.31–7.21 (*m*, 2H), 4.17 (*s*, 2H). ¹³C NMR (100 MHz, CDCl₃) δ = 148.5, 138.8, 137.2, 129.6, 128.8, 128.7, 128.5, 126.6, 120.42, 119.6, 32.3 ppm. ESI-MS (*m/z*) calculated for C₁₅H₁₂N₄O₂ [*M* + H]⁺ 281.1038, found 281.1039.

7. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 4. The carbon-bound H atoms were placed in calculated positions (C—H = 0.93–0.97 Å) and were included in the refinement in the riding-model approximation, with $U_{\text{iso}}(\text{H})$ set to $1.2U_{\text{eq}}(\text{C})$.

Table 4

Experimental details.

Crystal data	
Chemical formula	C ₁₅ H ₁₂ N ₄ O ₂
M_r	280.29
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, b, c (Å)	5.1962 (1), 10.7814 (3), 24.0067 (6)
β (°)	90.256 (2)
V (Å ³)	1344.90 (6)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	0.10
Crystal size (mm)	0.46 × 0.26 × 0.14
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (SADABS; Sheldrick, 1996)
$T_{\text{min}}, T_{\text{max}}$	0.695, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9104, 2450, 1881
R_{int}	0.023
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.603
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.040, 0.106, 1.06
No. of reflections	2450
No. of parameters	190
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.16, -0.18

Computer programs: APEX2 and SAINT (Bruker, 2009), SIR2014 (Burla *et al.*, 2015), SHELXL2014 (Sheldrick, 2015), ORTEP-3 for Windows (Farrugia, 2012), DIAMOND (Brandenburg, 2006), MarvinSketch (ChemAxon, 2010) and publCIF (Westrip, 2010).

Acknowledgements

We thank Professor Regina H. A. Santos from IQSC-USP for the X-ray data collection.

Funding information

The Brazilian agency National Council for Scientific and Technological Development, CNPq, is gratefully acknowledged for fellowships to JZ-S (305626/2013–2) and MWP (13/02311–3). AA acknowledges CNPQ–Twas for a scholarship.

References

- Ali, A., Corrêa, A. G., Alves, D., Zukerman-Schpector, J., Westermann, B., Ferreira, M. A. B. & Paixão, M. W. (2014). *Chem. Commun.* **50**, 11926–11929.
- Brandenburg, K. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
- Bruker (2009). *APEX2* and *SAINTE*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Burla, M. C., Caliendo, R., Carrozzini, B., Cascarano, G. L., Cuocci, C., Giacovazzo, C., Mallamo, M., Mazzone, A. & Polidori, G. (2015). *J. Appl. Cryst.* **48**, 306–309.
- ChemAxon (2010). *Marvinsketch*. <http://www.chemaxon.com>.
- Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
- Golas, P. L. & Matyjaszewski, K. (2010). *Chem. Soc. Rev.* **39**, 1338–1354.
- Holub, J. M. & Kirshenbaum, K. (2010). *Chem. Soc. Rev.* **39**, 1325–1337.
- Huang, L., Massa, L. & Karle, J. (2008). *Proc. Natl Acad. Sci.* **105**, 13720–13723.

- Jewett, J. C. & Bertozzi, C. R. (2010). *Chem. Soc. Rev.* **39**, 1272–1279.
- Muhammad, N. A., Khawaja, A. Y., Tariq, M., Fatima, W., Muhammad, H. K., Tahir, M. N., Safeena, Z. & Shaista, A. (2015). *Chin. J. Struct. Chem.* **34**, 1830–1840.
- Qin, A., Lam, J. W. Y. & Tang, B. Z. (2010). *Chem. Soc. Rev.* **39**, 2522–2544.
- Sarode, P. B., Bahekar, S. P. & Chandak, H. S. (2016). *Synlett*, **27**, 2681–2684.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (2015). *Acta Cryst.* **C71**, 3–8.
- Thirumurugan, P., Matosiuk, D. & Jozwiak, K. (2013). *Chem. Rev.* **113**, 4905–4979.
- Tron, G. C., Pirali, T., Billington, R. A., Canonico, P. L., Sorba, G. & Genazzani, A. A. (2008). *Med. Res. Rev.* **28**, 278–308.
- Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
- Wolff, S. K., Grimwood, D. J., McKinnon, J. J., Turner, M. J., Jayatilaka, D. & Spackman, M. A. (2012). University of Western Australia.
- Zukerman-Schpector, J., Prado, K. E., Name, L. L., Cella, R., Jotani, M. M. & Tiekink, E. R. T. (2017). *Acta Cryst.* **E73**, 918–924.

supporting information

Acta Cryst. (2017). E73, 1716-1720 [https://doi.org/10.1107/S2056989017014748]

4-Benzyl-1-(4-nitrophenyl)-1*H*-1,2,3-triazole: crystal structure and Hirshfeld analysis

Julio Zukerman-Schpector, Sofia Dallasta Pedroso, Lucas Sousa Madureira, Márcio Weber Paixão, Akbar Ali and Edward R. T. Tiekink

Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *S SAINT* (Bruker, 2009); data reduction: *S SAINT* (Bruker, 2009); program(s) used to solve structure: *SIR2014* (Burla *et al.*, 2015); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *MarvinSketch* (ChemAxon, 2010) and *publCIF* (Westrip, 2010).

4-Benzyl-1-(4-nitrophenyl)-1*H*-1,2,3-triazole

Crystal data

$C_{15}H_{12}N_4O_2$

$M_r = 280.29$

Monoclinic, $P2_1/c$

$a = 5.1962$ (1) Å

$b = 10.7814$ (3) Å

$c = 24.0067$ (6) Å

$\beta = 90.256$ (2)°

$V = 1344.90$ (6) Å³

$Z = 4$

$F(000) = 584$

$D_x = 1.384$ Mg m⁻³

Melting point = 371–373 K

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2937 reflections

$\theta = 3.2$ – 25.0 °

$\mu = 0.10$ mm⁻¹

$T = 293$ K

Irregular, yellow

$0.46 \times 0.26 \times 0.14$ mm

Data collection

Bruker APEXII CCD

diffractometer

φ and ω scans

Absorption correction: multi-scan

(SADABS; Sheldrick, 1996)

$T_{\min} = 0.695$, $T_{\max} = 0.745$

9104 measured reflections

2450 independent reflections

1881 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.023$

$\theta_{\max} = 25.4$ °, $\theta_{\min} = 1.7$ °

$h = -6$ → 6

$k = -12$ → 12

$l = -28$ → 28

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.040$

$wR(F^2) = 0.106$

$S = 1.06$

2450 reflections

190 parameters

0 restraints

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0383P)^2 + 0.3766P]$

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

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.16$ e Å⁻³

$\Delta\rho_{\min} = -0.18$ e Å⁻³

Special details

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.6006 (3)	-0.10629 (18)	0.84523 (7)	0.0532 (4)
C2	0.4648 (3)	-0.01241 (18)	0.86767 (6)	0.0531 (4)
H2	0.3030	0.0154	0.8566	0.064*
C3	0.5294 (4)	-0.1916 (2)	0.79835 (7)	0.0672 (5)
H3A	0.3644	-0.1662	0.7832	0.081*
H3B	0.5100	-0.2750	0.8129	0.081*
C4	0.7242 (3)	-0.19387 (16)	0.75201 (7)	0.0519 (4)
C5	0.7534 (4)	-0.09304 (18)	0.71743 (8)	0.0646 (5)
H5	0.6472	-0.0244	0.7220	0.078*
C6	0.9359 (4)	-0.0918 (2)	0.67636 (8)	0.0762 (6)
H6	0.9520	-0.0224	0.6536	0.091*
C7	1.0933 (4)	-0.1905 (3)	0.66847 (9)	0.0803 (7)
H7	1.2195	-0.1884	0.6411	0.096*
C8	1.0641 (4)	-0.2926 (3)	0.70110 (10)	0.0836 (7)
H8	1.1682	-0.3616	0.6954	0.100*
C9	0.8791 (4)	-0.29477 (19)	0.74304 (8)	0.0695 (5)
H9	0.8607	-0.3651	0.7651	0.083*
C10	0.5585 (3)	0.13033 (15)	0.94757 (6)	0.0444 (4)
C11	0.3575 (3)	0.21075 (18)	0.93671 (7)	0.0577 (5)
H11	0.2615	0.2024	0.9041	0.069*
C12	0.2992 (4)	0.30319 (18)	0.97405 (8)	0.0627 (5)
H12	0.1625	0.3569	0.9674	0.075*
C13	0.4468 (3)	0.31461 (16)	1.02137 (7)	0.0541 (4)
C14	0.6508 (3)	0.23726 (17)	1.03240 (7)	0.0562 (4)
H14	0.7494	0.2478	1.0645	0.067*
C15	0.7071 (3)	0.14397 (17)	0.99526 (6)	0.0511 (4)
H15	0.8439	0.0904	1.0021	0.061*
N1	0.6118 (2)	0.03310 (13)	0.90952 (5)	0.0451 (3)
N2	0.8341 (3)	-0.03164 (15)	0.91281 (6)	0.0583 (4)
N3	0.8269 (3)	-0.11635 (15)	0.87374 (6)	0.0628 (4)
N4	0.3812 (4)	0.41242 (16)	1.06168 (7)	0.0729 (5)
O1	0.1984 (4)	0.47864 (19)	1.05159 (8)	0.1170 (7)
O2	0.5137 (4)	0.42327 (16)	1.10290 (7)	0.1031 (6)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0419 (9)	0.0744 (12)	0.0432 (8)	-0.0121 (8)	0.0010 (7)	0.0016 (8)
C2	0.0367 (8)	0.0806 (13)	0.0420 (8)	-0.0047 (8)	-0.0035 (7)	0.0027 (8)

C3	0.0609 (11)	0.0851 (14)	0.0556 (10)	-0.0213 (10)	0.0005 (9)	-0.0091 (10)
C4	0.0513 (10)	0.0585 (11)	0.0458 (8)	-0.0051 (8)	-0.0084 (7)	-0.0099 (8)
C5	0.0728 (13)	0.0615 (12)	0.0596 (11)	0.0065 (10)	0.0030 (9)	-0.0019 (9)
C6	0.0879 (15)	0.0881 (16)	0.0526 (11)	-0.0147 (13)	0.0046 (10)	-0.0034 (10)
C7	0.0646 (13)	0.122 (2)	0.0539 (11)	-0.0053 (14)	0.0001 (10)	-0.0310 (13)
C8	0.0712 (14)	0.0994 (18)	0.0800 (14)	0.0278 (13)	-0.0165 (12)	-0.0410 (14)
C9	0.0803 (14)	0.0621 (12)	0.0660 (12)	0.0053 (11)	-0.0214 (10)	-0.0076 (10)
C10	0.0371 (8)	0.0573 (10)	0.0389 (8)	-0.0030 (7)	0.0038 (6)	0.0098 (7)
C11	0.0495 (10)	0.0753 (13)	0.0483 (9)	0.0074 (9)	-0.0065 (8)	0.0056 (9)
C12	0.0561 (11)	0.0688 (12)	0.0631 (11)	0.0122 (9)	0.0009 (9)	0.0083 (9)
C13	0.0581 (10)	0.0533 (10)	0.0509 (9)	-0.0034 (8)	0.0107 (8)	0.0048 (8)
C14	0.0568 (10)	0.0665 (11)	0.0454 (8)	-0.0074 (9)	-0.0031 (8)	0.0035 (8)
C15	0.0439 (9)	0.0627 (11)	0.0468 (9)	0.0007 (8)	-0.0050 (7)	0.0048 (8)
N1	0.0337 (7)	0.0630 (9)	0.0384 (6)	0.0005 (6)	-0.0008 (5)	0.0050 (6)
N2	0.0415 (8)	0.0786 (10)	0.0547 (8)	0.0099 (7)	-0.0091 (6)	-0.0088 (8)
N3	0.0518 (9)	0.0784 (11)	0.0582 (9)	0.0064 (8)	-0.0062 (7)	-0.0122 (8)
N4	0.0873 (13)	0.0647 (11)	0.0668 (11)	-0.0013 (10)	0.0104 (10)	-0.0005 (9)
O1	0.1292 (16)	0.1118 (14)	0.1100 (13)	0.0544 (13)	-0.0054 (12)	-0.0279 (11)
O2	0.1333 (15)	0.0942 (12)	0.0817 (11)	0.0065 (11)	-0.0145 (11)	-0.0274 (9)

Geometric parameters (Å, °)

C1—C2	1.347 (2)	C9—H9	0.9300
C1—N3	1.362 (2)	C10—C11	1.382 (2)
C1—C3	1.499 (2)	C10—C15	1.386 (2)
C2—N1	1.3516 (19)	C10—N1	1.418 (2)
C2—H2	0.9300	C11—C12	1.375 (3)
C3—C4	1.507 (2)	C11—H11	0.9300
C3—H3A	0.9700	C12—C13	1.373 (2)
C3—H3B	0.9700	C12—H12	0.9300
C4—C9	1.371 (3)	C13—C14	1.374 (2)
C4—C5	1.377 (2)	C13—N4	1.472 (2)
C5—C6	1.371 (3)	C14—C15	1.376 (2)
C5—H5	0.9300	C14—H14	0.9300
C6—C7	1.356 (3)	C15—H15	0.9300
C6—H6	0.9300	N1—N2	1.3516 (18)
C7—C8	1.360 (3)	N2—N3	1.310 (2)
C7—H7	0.9300	N4—O2	1.209 (2)
C8—C9	1.395 (3)	N4—O1	1.212 (2)
C8—H8	0.9300		
C2—C1—N3	108.14 (15)	C4—C9—H9	119.8
C2—C1—C3	129.31 (16)	C8—C9—H9	119.8
N3—C1—C3	122.53 (17)	C11—C10—C15	120.48 (16)
C1—C2—N1	105.95 (14)	C11—C10—N1	119.46 (14)
C1—C2—H2	127.0	C15—C10—N1	120.06 (14)
N1—C2—H2	127.0	C12—C11—C10	120.02 (15)
C1—C3—C4	113.59 (14)	C12—C11—H11	120.0

C1—C3—H3A	108.8	C10—C11—H11	120.0
C4—C3—H3A	108.8	C13—C12—C11	118.71 (17)
C1—C3—H3B	108.8	C13—C12—H12	120.6
C4—C3—H3B	108.8	C11—C12—H12	120.6
H3A—C3—H3B	107.7	C12—C13—C14	122.19 (17)
C9—C4—C5	117.75 (18)	C12—C13—N4	118.55 (17)
C9—C4—C3	121.69 (18)	C14—C13—N4	119.26 (16)
C5—C4—C3	120.56 (17)	C13—C14—C15	119.00 (16)
C6—C5—C4	121.32 (19)	C13—C14—H14	120.5
C6—C5—H5	119.3	C15—C14—H14	120.5
C4—C5—H5	119.3	C14—C15—C10	119.57 (16)
C7—C6—C5	120.8 (2)	C14—C15—H15	120.2
C7—C6—H6	119.6	C10—C15—H15	120.2
C5—C6—H6	119.6	C2—N1—N2	109.62 (14)
C6—C7—C8	119.1 (2)	C2—N1—C10	129.48 (13)
C6—C7—H7	120.5	N2—N1—C10	120.88 (12)
C8—C7—H7	120.5	N3—N2—N1	107.26 (13)
C7—C8—C9	120.5 (2)	N2—N3—C1	109.03 (15)
C7—C8—H8	119.7	O2—N4—O1	123.3 (2)
C9—C8—H8	119.7	O2—N4—C13	118.35 (19)
C4—C9—C8	120.5 (2)	O1—N4—C13	118.30 (18)
N3—C1—C2—N1	0.06 (19)	N4—C13—C14—C15	178.33 (15)
C3—C1—C2—N1	178.62 (16)	C13—C14—C15—C10	0.3 (3)
C2—C1—C3—C4	125.1 (2)	C11—C10—C15—C14	1.0 (2)
N3—C1—C3—C4	-56.5 (2)	N1—C10—C15—C14	-178.83 (15)
C1—C3—C4—C9	108.8 (2)	C1—C2—N1—N2	-0.02 (18)
C1—C3—C4—C5	-70.5 (2)	C1—C2—N1—C10	-178.32 (15)
C9—C4—C5—C6	-1.8 (3)	C11—C10—N1—C2	-14.9 (2)
C3—C4—C5—C6	177.62 (17)	C15—C10—N1—C2	164.92 (16)
C4—C5—C6—C7	0.2 (3)	C11—C10—N1—N2	166.96 (15)
C5—C6—C7—C8	1.5 (3)	C15—C10—N1—N2	-13.2 (2)
C6—C7—C8—C9	-1.6 (3)	C2—N1—N2—N3	-0.03 (18)
C5—C4—C9—C8	1.7 (3)	C10—N1—N2—N3	178.44 (14)
C3—C4—C9—C8	-177.68 (16)	N1—N2—N3—C1	0.07 (19)
C7—C8—C9—C4	-0.1 (3)	C2—C1—N3—N2	-0.1 (2)
C15—C10—C11—C12	-1.7 (3)	C3—C1—N3—N2	-178.76 (16)
N1—C10—C11—C12	178.13 (16)	C12—C13—N4—O2	-179.00 (18)
C10—C11—C12—C13	1.0 (3)	C14—C13—N4—O2	1.6 (3)
C11—C12—C13—C14	0.3 (3)	C12—C13—N4—O1	0.4 (3)
C11—C12—C13—N4	-179.03 (16)	C14—C13—N4—O1	-178.99 (19)
C12—C13—C14—C15	-1.0 (3)		

Hydrogen-bond geometry (Å, °)

Cg1—Cg3 are the centroids of the N1—N3/C1/C2, C4—C9 and C10—C15 rings, respectively.

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C3—H3B \cdots O2 ⁱ	0.97	2.58	3.452 (3)	150

C3—H3A...Cg2 ⁱⁱ	0.97	2.96	3.857 (2)	154
C8—H8...Cg1 ⁱⁱⁱ	0.93	2.86	3.665 (3)	146
N4—O1...Cg3 ^{iv}	1.21 (1)	3.67 (1)	4.1254 (19)	103 (1)

Symmetry codes: (i) $-x+1, -y, -z+2$; (ii) $x-1, y, z$; (iii) $-x+2, y-1/2, -z+3/2$; (iv) $-x+1, -y+1, -z+2$.