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6,6-Dibenzyltetrazolo[1,5-*a*]pyrimidine-5,7(4*H*,6*H*)-dione

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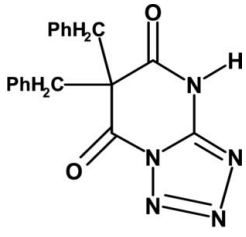
Key indicators: single-crystal X-ray study; T = 297 K; mean σ(C–C) = 0.004 Å; R factor = 0.052; wR factor = 0.122; data-to-parameter ratio = 10.3.

The title compound, $C_{18}H_{15}N_5O_2$, exhibits a conformation in which the benzyl groups are folded symmetrically towards the tetrazole–pyrimidine–dione group. Molecules related by an inversion centre form dimers *via* intermolecular N—H···O hydrogen bonds. These dimers are linked to each other through weak C—H···N hydrogen bonds.

Related literature

For related literature, see: Baruah *et al.* (2005); Johnstone *et al.* (1980); Maslak *et al.* (1999); Meijer *et al.* (2005); Zimmerman *et al.* (2002).



Experimental

Crystal data

$C_{18}H_{15}N_5O_2$
M_r = 333.35
Orthorhombic, *Pbca*
a = 8.6247 (13) Å
b = 16.777 (3) Å
c = 22.950 (4) Å
V = 3320.8 (9) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 297 (2) K
0.41 × 0.10 × 0.04 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2003)
T_{min} = 0.963, T_{max} = 0.997
15340 measured reflections
2932 independent reflections
1813 reflections with $I > 2\sigma(I)$
R_{int} = 0.074

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.122
S = 1.01
2932 reflections
286 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15···N2^{i}	0.98 (3)	2.73 (3)	3.368 (4)	123.0 (19)
C12—H12B···N3^{ii}	0.95 (2)	2.67 (3)	3.542 (4)	152.8 (18)
C9—H9···N4^{iii}	0.97 (3)	2.68 (3)	3.501 (4)	143 (2)
C5—H5B···N4^{iv}	1.00 (2)	2.71 (3)	3.682 (4)	165.8 (19)
N1—H1···O1^{v}	0.89 (3)	1.89 (4)	2.774 (3)	175 (3)

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

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXTL* (Bruker, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CF2114).

References

Baruah, P. K., Gonnade, R., Phalgune, U. D. & Sanjayan, G. J. (2005). *J. Org. Chem.* **70**, 6461–6467.
Bruker (2003). *SADABS* (Version 2.05), *SMART* (Version 5.631), *SAINT* (Version 6.45) and *SHELXTL* (Version 6.14). Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Johnstone, R. A. W., Tuli, D. & Rose, M. E. (1980). *J. Chem. Res. Synop.* **9**, 283.
Macrae, C. F., Edgington, P. R., McCabe, P., Pidcock, E., Shields, G. P., Taylor, R., Towler, M. & van de Streek, J. (2006). *J. Appl. Cryst.* **39**, 453–457.
Maslak, P., Varadarajan, S. & Burkey, J. D. (1999). *J. Org. Chem.* **64**, 8201–8209.
Meijer, E. W., Ligthart, G. B. W. L., Ohkawa, H. & Sijbesma, R. P. (2005). *J. Am. Chem. Soc.* **127**, 810–811.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Zimmerman, S. C., Corbin, P. S., Lawless, L. J., Li, Z., Ma, Y. & Witmer, M. J. (2002). *Proc. Natl Acad. Sci. USA*, **99**, 5099–5104.

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supplementary materials

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6,6-Dibenzyltetrazolo[1,5-*a*]pyrimidine-5,7(4*H*,6*H*)-dione

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Comment

Heterocycle-based self-assembling systems capable of forming two-, three- and four-centered hydrogen bonds are gaining interest in designing functional solids due to their high dimerization constant (Zimmerman *et al.,* 2002; Meijer *et al.,* 2005; Baruah *et al.*, 2005). The tetrazole-based title compound (I) has been synthesized and we report here its crystal structure.

The title molecule adopts a 'bat-like' conformation (Fig. 1). The central tetrazole-pyrimidine-dione group is approximately planar. Molecules of (I) form centrosymmetric dimers (Fig. 2) *via* intermolecular N—H···O hydrogen bonds (Table 1) in which tetrazole-pyrimidine-dione groups are coplanar and the benzyl groups are approximately perpendicular to this plane.

The molecular packing viewed down the *a* axis (Fig. 3) shows the association of the centrosymmetric dimers *via* C—H···N contacts (Table 1). The C9—H9···N4^{iii} and C15—H15···N2^{i} interactions link the centrosymmetric dimers along the *b* axis, whereas along the *c* axis these dimers are associated *via* the C5—H5B···N4^{iv} contact.

Experimental

Dibenzyl diethylmalonate and dibenzyl malonic acid were synthesized according to the literature procedure (Maslak *et al.*, 1999; Johnstone *et al.,* 1980). To a solution of dibenzyl malonic acid (2.85 g, 10 mmol, 1 equiv.) in dry dichloromethane (10 ml) at 273 K, oxalyl chloride (3.5 ml, 40 mmol, 4 equiv.) was added along with a catalytic amount of *N*,*N*-dimethylformamide (DMF). After stirring the reaction mixture at room temperature for 2 h, the solvent was removed under reduced pressure. The resulting diacid chloride was dissolved in dry DMF (5 ml) and added to a solution containing 5-aminotetrazole (1.27 g, 10 mmol, 1 equiv.) and *N*,*N*-diisopropylethylamine (5.2 ml, 30 mmol, 3 equiv.) in dry DMF (5 ml) maintained at 253 K. The reaction mixture was stirred for 4 h at room temperature and poured into water. The usual work-up and purification of the crude product by column chromatography afforded a white solid (1.95 g, 81.5%). Colorless single crystals suitable for X-ray diffraction were obtained by slow evaporation of a solution in a dichloromethane-light petroleum ether mixture at room temperature.

Refinement

All the H atoms were located in a difference Fourier map and refined freely.

Figures

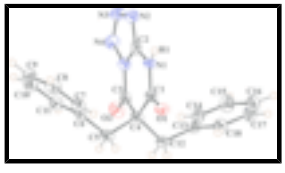

Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms.

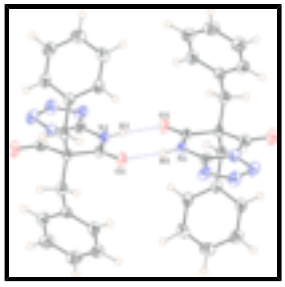

Fig. 2. Centrosymmetric dimeric association of molecules of (I), connected by N—H···O hydrogen bonds shown as dashed lines.

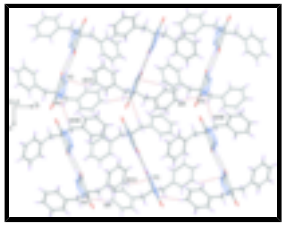

Fig. 3. A packing diagram of (I), viewed down the *a* axis, showing linking of the centrosymmetric dimers through C—H···N hydrogen bonds depicted by red dashed lines.

6,6-Dibenzyltetrazolo[1,5-*a*]pyrimidine-5,7(4*H*,6*H*)-dione

Crystal data

$C_{18}H_{15}N_5O_2$	F_{000} = 1392
M_r = 333.35	D_x = 1.334 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 1821 reflections
a = 8.6247 (13) Å	θ = 2.4–21.4º
b = 16.777 (3) Å	μ = 0.09 mm^{-1}
c = 22.950 (4) Å	*T* = 297 (2) K
V = 3320.8 (9) Å^3	Needle, colorless
Z = 8	0.41 × 0.10 × 0.04 mm

Data collection

CCD area-detector diffractometer	2932 independent reflections
Radiation source: fine-focus sealed tube	1813 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.074
T = 297(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Bruker, 2003)	*h* = −10→10
T_{min} = 0.963, T_{max} = 0.997	*k* = −17→19
15340 measured reflections	*l* = −20→27

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.052$	All H-atom parameters refined
$wR(F^2) = 0.122$	$w = 1/[\sigma^2(F_o^2) + (0.0534P)^2 + 0.911P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} < 0.001$
2932 reflections	$\Delta\rho_{max} = 0.19$ e Å^{-3}
286 parameters	$\Delta\rho_{min} = -0.23$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > 2$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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	−0.1488 (2)	0.03404 (11)	0.54832 (7)	0.0354 (5)
O2	0.0857 (2)	0.13057 (11)	0.72322 (8)	0.0453 (5)
N1	0.1102 (2)	0.03592 (14)	0.56024 (9)	0.0286 (5)
N2	0.3838 (3)	0.03595 (14)	0.58267 (10)	0.0399 (6)
N3	0.4617 (3)	0.05786 (14)	0.63174 (10)	0.0423 (6)
N4	0.3698 (3)	0.08262 (14)	0.67263 (10)	0.0420 (6)
N5	0.2222 (2)	0.07682 (13)	0.64897 (9)	0.0334 (6)
C1	−0.0375 (3)	0.04826 (15)	0.57957 (11)	0.0286 (6)
C2	0.2361 (3)	0.04863 (15)	0.59512 (11)	0.0314 (6)
C3	0.0833 (3)	0.09921 (15)	0.67621 (12)	0.0322 (6)
C4	−0.0634 (3)	0.07811 (15)	0.64204 (10)	0.0273 (6)
C5	−0.1472 (3)	0.00954 (16)	0.67624 (12)	0.0309 (7)
C6	−0.0575 (3)	−0.06689 (15)	0.68050 (10)	0.0286 (6)
C7	−0.0797 (3)	−0.12794 (16)	0.64032 (12)	0.0347 (7)
C8	0.0003 (4)	−0.19929 (18)	0.64508 (13)	0.0430 (8)
C9	0.1036 (4)	−0.21058 (19)	0.69051 (14)	0.0447 (8)
C10	0.1284 (4)	−0.15038 (18)	0.73039 (14)	0.0436 (8)
C11	0.0484 (3)	−0.07930 (18)	0.72570 (12)	0.0366 (7)
C12	−0.1717 (3)	0.15218 (17)	0.64069 (12)	0.0318 (7)
C13	−0.1120 (3)	0.22087 (16)	0.60477 (11)	0.0317 (6)
C14	−0.0059 (4)	0.27493 (18)	0.62691 (13)	0.0409 (7)
C15	0.0449 (4)	0.33920 (19)	0.59442 (15)	0.0506 (9)

C16	−0.0121 (4)	0.3509 (2)	0.53849 (14)	0.0501 (8)
C17	−0.1148 (4)	0.29751 (19)	0.51558 (13)	0.0473 (8)
C18	−0.1652 (4)	0.23301 (19)	0.54796 (12)	0.0407 (7)
H1	0.127 (4)	0.0115 (19)	0.5266 (15)	0.072 (11)*
H7	−0.158 (3)	−0.1225 (16)	0.6105 (11)	0.041 (8)*
H8	−0.014 (3)	−0.2450 (18)	0.6191 (13)	0.059 (9)*
H9	0.159 (3)	−0.2605 (16)	0.6925 (11)	0.042 (8)*
H10	0.199 (3)	−0.1603 (15)	0.7625 (11)	0.041 (8)*
H11	0.060 (3)	−0.0377 (15)	0.7524 (12)	0.036 (8)*
H14	0.033 (3)	0.2692 (17)	0.6642 (12)	0.051 (9)*
H15	0.118 (3)	0.3780 (17)	0.6111 (11)	0.043 (8)*
H16	0.021 (3)	0.3982 (17)	0.5183 (13)	0.057 (9)*
H17	−0.160 (3)	0.3020 (17)	0.4752 (13)	0.057 (9)*
H18	−0.232 (3)	0.1955 (14)	0.5325 (10)	0.030 (7)*
H5A	−0.242 (3)	0.0023 (13)	0.6565 (10)	0.027 (7)*
H12A	−0.187 (3)	0.1670 (14)	0.6826 (11)	0.033 (7)*
H5B	−0.163 (3)	0.0319 (13)	0.7160 (11)	0.029 (7)*
H12B	−0.269 (3)	0.1353 (14)	0.6252 (10)	0.024 (6)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0256 (10)	0.0551 (12)	0.0254 (9)	0.0020 (9)	−0.0013 (8)	−0.0077 (9)
O2	0.0500 (13)	0.0565 (13)	0.0296 (11)	−0.0135 (10)	−0.0050 (9)	−0.0048 (10)
N1	0.0203 (12)	0.0438 (14)	0.0216 (11)	0.0002 (10)	−0.0002 (9)	−0.0031 (10)
N2	0.0284 (14)	0.0544 (15)	0.0370 (13)	0.0011 (11)	−0.0047 (11)	0.0029 (12)
N3	0.0257 (14)	0.0562 (16)	0.0451 (15)	−0.0016 (11)	−0.0060 (12)	−0.0055 (13)
N4	0.0317 (15)	0.0536 (15)	0.0406 (14)	−0.0056 (12)	−0.0114 (12)	0.0014 (12)
N5	0.0290 (14)	0.0406 (13)	0.0308 (13)	−0.0029 (11)	−0.0022 (10)	0.0017 (11)
C1	0.0292 (16)	0.0353 (15)	0.0212 (13)	−0.0012 (12)	−0.0001 (12)	0.0004 (12)
C2	0.0377 (18)	0.0318 (15)	0.0248 (14)	−0.0047 (13)	−0.0024 (12)	0.0060 (12)
C3	0.0354 (17)	0.0293 (15)	0.0318 (15)	−0.0039 (12)	0.0054 (13)	0.0055 (13)
C4	0.0247 (15)	0.0365 (15)	0.0207 (12)	−0.0020 (12)	0.0028 (11)	−0.0034 (12)
C5	0.0268 (16)	0.0438 (17)	0.0222 (14)	−0.0059 (13)	0.0031 (13)	−0.0061 (13)
C6	0.0242 (15)	0.0378 (15)	0.0237 (13)	−0.0074 (12)	0.0042 (11)	0.0018 (12)
C7	0.0314 (17)	0.0429 (18)	0.0298 (15)	−0.0081 (14)	−0.0009 (13)	−0.0043 (13)
C8	0.0441 (19)	0.0410 (18)	0.0439 (17)	−0.0056 (15)	0.0018 (15)	−0.0110 (15)
C9	0.0374 (18)	0.0400 (18)	0.057 (2)	0.0008 (16)	0.0023 (15)	0.0029 (17)
C10	0.0365 (19)	0.0483 (19)	0.0462 (18)	−0.0067 (15)	−0.0112 (16)	0.0048 (16)
C11	0.0378 (18)	0.0416 (17)	0.0303 (15)	−0.0081 (14)	−0.0028 (13)	−0.0033 (14)
C12	0.0261 (16)	0.0416 (17)	0.0278 (16)	0.0004 (13)	0.0037 (12)	−0.0023 (13)
C13	0.0300 (15)	0.0359 (15)	0.0293 (14)	0.0065 (13)	0.0033 (12)	−0.0024 (12)
C14	0.0439 (19)	0.0421 (18)	0.0367 (16)	0.0009 (15)	−0.0073 (15)	0.0020 (15)
C15	0.052 (2)	0.0407 (19)	0.059 (2)	−0.0102 (16)	−0.0100 (17)	0.0057 (17)
C16	0.056 (2)	0.0455 (19)	0.049 (2)	0.0007 (17)	0.0091 (17)	0.0103 (17)
C17	0.061 (2)	0.049 (2)	0.0325 (17)	0.0101 (17)	−0.0002 (16)	0.0018 (16)
C18	0.0422 (18)	0.0431 (18)	0.0367 (17)	0.0000 (15)	−0.0055 (14)	−0.0038 (15)

Geometric parameters (Å, °)

O1—C1	1.222 (3)	C8—C9	1.384 (4)
O2—C3	1.201 (3)	C8—H8	0.98 (3)
N1—C1	1.364 (3)	C9—C10	1.380 (4)
N1—C2	1.366 (3)	C9—H9	0.97 (3)
N1—H1	0.89 (3)	C10—C11	1.382 (4)
N2—C2	1.323 (3)	C10—H10	0.97 (3)
N2—N3	1.361 (3)	C11—H11	0.93 (3)
N3—N4	1.297 (3)	C12—C13	1.507 (4)
N4—N5	1.388 (3)	C12—H12A	1.00 (2)
N5—C2	1.329 (3)	C12—H12B	0.95 (2)
N5—C3	1.402 (3)	C13—C14	1.385 (4)
C1—C4	1.535 (3)	C13—C18	1.397 (4)
C3—C4	1.530 (4)	C14—C15	1.382 (4)
C4—C12	1.555 (4)	C14—H14	0.92 (3)
C4—C5	1.569 (4)	C15—C16	1.388 (4)
C5—C6	1.501 (4)	C15—H15	0.98 (3)
C5—H5A	0.94 (3)	C16—C17	1.366 (4)
C5—H5B	1.00 (2)	C16—H16	0.96 (3)
C6—C7	1.391 (3)	C17—C18	1.383 (4)
C6—C11	1.397 (4)	C17—H17	1.01 (3)
C7—C8	1.386 (4)	C18—H18	0.92 (2)
C7—H7	0.96 (3)		
C1—N1—C2	121.9 (2)	C9—C8—C7	119.9 (3)
C1—N1—H1	120 (2)	C9—C8—H8	115.7 (17)
C2—N1—H1	117 (2)	C7—C8—H8	124.4 (18)
C2—N2—N3	104.6 (2)	C10—C9—C8	120.0 (3)
N4—N3—N2	112.6 (2)	C10—C9—H9	121.7 (16)
N3—N4—N5	104.8 (2)	C8—C9—H9	118.3 (16)
C2—N5—N4	107.8 (2)	C9—C10—C11	120.2 (3)
C2—N5—C3	126.0 (2)	C9—C10—H10	118.3 (15)
N4—N5—C3	126.2 (2)	C11—C10—H10	121.4 (15)
O1—C1—N1	120.9 (2)	C10—C11—C6	120.8 (3)
O1—C1—C4	119.8 (2)	C10—C11—H11	122.8 (16)
N1—C1—C4	119.3 (2)	C6—C11—H11	116.4 (16)
N2—C2—N5	110.2 (2)	C13—C12—C4	114.6 (2)
N2—C2—N1	127.9 (2)	C13—C12—H12A	112.2 (14)
N5—C2—N1	121.9 (2)	C4—C12—H12A	104.9 (14)
O2—C3—N5	120.3 (2)	C13—C12—H12B	108.8 (14)
O2—C3—C4	125.1 (2)	C4—C12—H12B	107.3 (14)
N5—C3—C4	114.6 (2)	H12A—C12—H12B	109 (2)
C3—C4—C1	115.7 (2)	C14—C13—C18	117.6 (3)
C3—C4—C12	108.8 (2)	C14—C13—C12	121.7 (2)
C1—C4—C12	109.3 (2)	C18—C13—C12	120.6 (3)
C3—C4—C5	107.1 (2)	C15—C14—C13	121.5 (3)
C1—C4—C5	107.2 (2)	C15—C14—H14	117.8 (18)
C12—C4—C5	108.6 (2)	C13—C14—H14	120.7 (18)

C6—C5—C4	115.0 (2)	C14—C15—C16	119.8 (3)
C6—C5—H5A	111.6 (14)	C14—C15—H15	120.6 (15)
C4—C5—H5A	104.7 (14)	C16—C15—H15	119.5 (15)
C6—C5—H5B	109.4 (14)	C17—C16—C15	119.5 (3)
C4—C5—H5B	104.2 (13)	C17—C16—H16	123.2 (18)
H5A—C5—H5B	112 (2)	C15—C16—H16	117.2 (18)
C7—C6—C11	118.2 (3)	C16—C17—C18	120.7 (3)
C7—C6—C5	121.0 (2)	C16—C17—H17	123.8 (17)
C11—C6—C5	120.8 (2)	C18—C17—H17	115.5 (18)
C8—C7—C6	121.0 (3)	C17—C18—C13	120.8 (3)
C8—C7—H7	119.0 (16)	C17—C18—H18	121.5 (15)
C6—C7—H7	119.8 (16)	C13—C18—H18	117.7 (15)
C2—N2—N3—N4	0.1 (3)	O1—C1—C4—C5	64.4 (3)
N2—N3—N4—N5	−0.1 (3)	N1—C1—C4—C5	−113.8 (3)
N3—N4—N5—C2	0.1 (3)	C3—C4—C5—C6	−63.6 (3)
N3—N4—N5—C3	−177.9 (2)	C1—C4—C5—C6	61.2 (3)
C2—N1—C1—O1	−177.6 (2)	C12—C4—C5—C6	179.1 (2)
C2—N1—C1—C4	0.6 (4)	C4—C5—C6—C7	−94.0 (3)
N3—N2—C2—N5	−0.1 (3)	C4—C5—C6—C11	87.3 (3)
N3—N2—C2—N1	−179.9 (2)	C11—C6—C7—C8	0.3 (4)
N4—N5—C2—N2	0.0 (3)	C5—C6—C7—C8	−178.4 (3)
C3—N5—C2—N2	178.0 (2)	C6—C7—C8—C9	0.3 (4)
N4—N5—C2—N1	179.8 (2)	C7—C8—C9—C10	−1.0 (5)
C3—N5—C2—N1	−2.1 (4)	C8—C9—C10—C11	1.1 (5)
C1—N1—C2—N2	177.0 (3)	C9—C10—C11—C6	−0.5 (4)
C1—N1—C2—N5	−2.8 (4)	C7—C6—C11—C10	−0.2 (4)
C2—N5—C3—O2	−173.4 (2)	C5—C6—C11—C10	178.5 (3)
N4—N5—C3—O2	4.3 (4)	C3—C4—C12—C13	68.6 (3)
C2—N5—C3—C4	8.3 (3)	C1—C4—C12—C13	−58.5 (3)
N4—N5—C3—C4	−174.0 (2)	C5—C4—C12—C13	−175.1 (2)
O2—C3—C4—C1	172.4 (2)	C4—C12—C13—C14	−82.6 (3)
N5—C3—C4—C1	−9.4 (3)	C4—C12—C13—C18	98.8 (3)
O2—C3—C4—C12	49.0 (3)	C18—C13—C14—C15	0.6 (4)
N5—C3—C4—C12	−132.7 (2)	C12—C13—C14—C15	−178.0 (3)
O2—C3—C4—C5	−68.2 (3)	C13—C14—C15—C16	0.7 (5)
N5—C3—C4—C5	110.0 (2)	C14—C15—C16—C17	−1.8 (5)
O1—C1—C4—C3	−176.3 (2)	C15—C16—C17—C18	1.5 (5)
N1—C1—C4—C3	5.5 (3)	C16—C17—C18—C13	−0.2 (5)
O1—C1—C4—C12	−53.1 (3)	C14—C13—C18—C17	−0.9 (4)
N1—C1—C4—C12	128.6 (2)	C12—C13—C18—C17	177.8 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15···N2^{i}	0.98 (3)	2.73 (3)	3.368 (4)	123.0 (19)
C12—H12B···N3^{ii}	0.95 (2)	2.67 (3)	3.542 (4)	152.8 (18)
C9—H9···N4^{iii}	0.97 (3)	2.68 (3)	3.501 (4)	143 (2)
C5—H5B···N4^{iv}	1.00 (2)	2.71 (3)	3.682 (4)	165.8 (19)

N1—H1···O1^{v}	0.89 (3)	1.89 (4)	2.774 (3)	175 (3)

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

Fig. 1

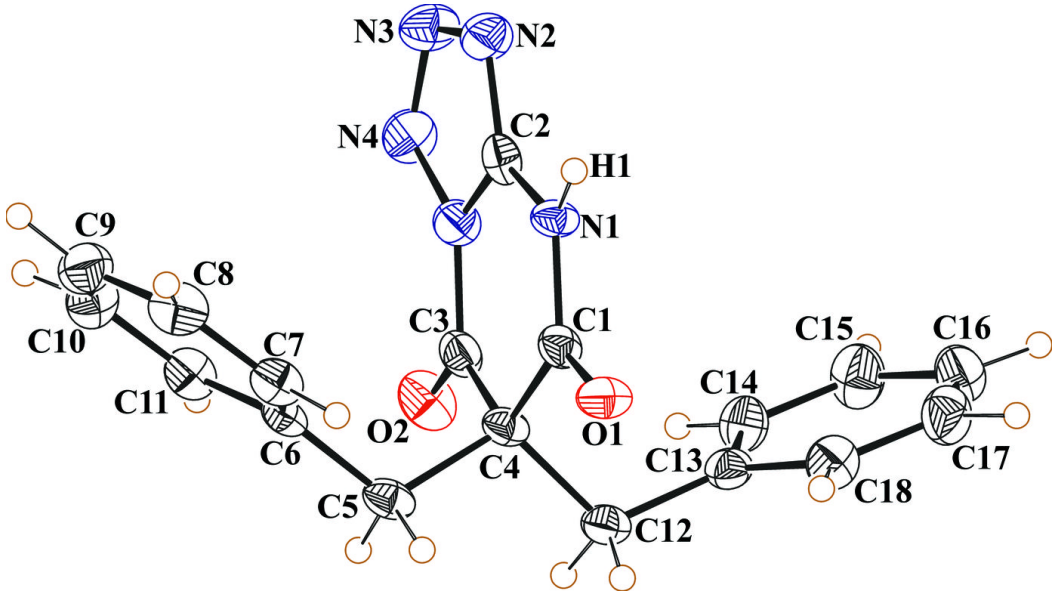

Fig. 2

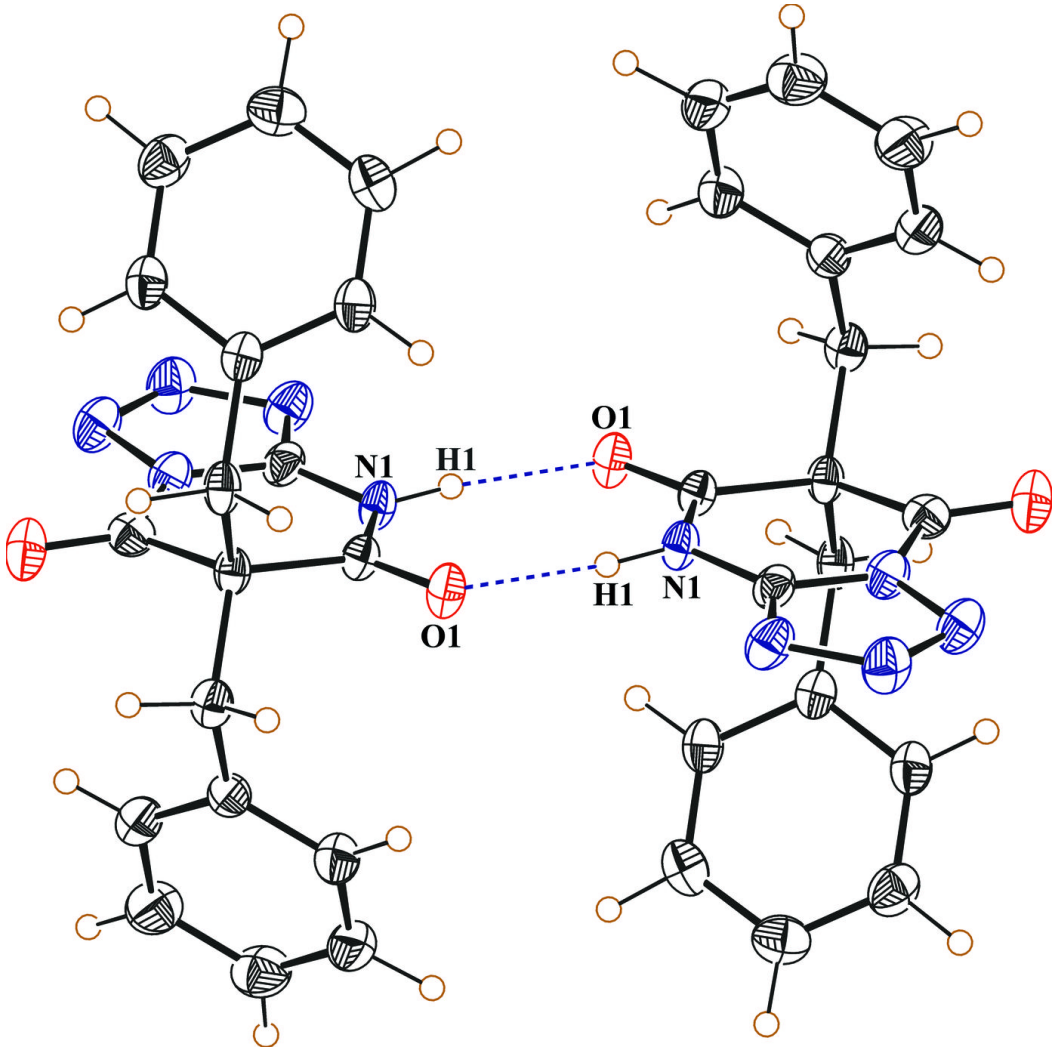

Fig. 3