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1-(4-Nitrophenyl)-2-({4-phenyl-5-[(*p*-tolyloxy)methyl]-4*H*-1,2,4-triazol-3-yl}sulfanyl)acetamide

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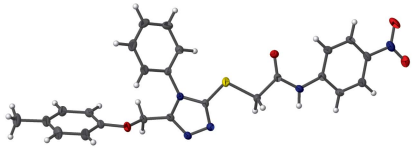
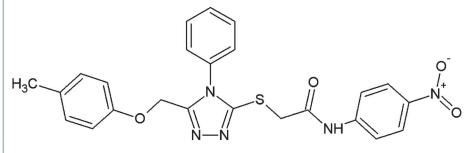
Structural data: full structural data are available from iucrdata.iucr.org

In the crystal structure of the title compound, $C_{24}H_{21}N_5O_4S$, centrosymmetric dimers with an $R_2^2(16)$ ring motif, lying in the (010) plane, are formed as a result of pairwise N—H···N hydrogen bonds. These dimers further interact through C—H···O and C—H···π interactions to construct a complex extended three-dimensional structure.

3D view



Chemical scheme



Structure description

There are a large number of drugs containing the 1,2,4-triazole nucleus in their structures including ribavirin (antiviral), rizatriptan (antimigraine), estazolam and alprazolam (anxiolytic), letrozole and anastrozole (breast cancer) (Godhani *et al.*, 2015). Others such as Itraconazole, Fluconazole and Posaconazole have been used for the treatment of fungal infections (Godhani *et al.*, 2015). As part of our studies in this area, we report the synthesis and crystal structure of the title compound.

The molecular conformation of the title compound (Fig. 1) is partially stabilized by an intramolecular C23—H23···O2 hydrogen bond (Table 1). The central 4*H*-1,2,4-triazole ring of the title molecule makes dihedral angles of 42.34 (9), 87.53 (9) and 58.39 (9)°, with the C6–C11 and C12–C17 benzene rings and the C18–C23 phenyl ring, respectively. All bond lengths and bond angles are within normal ranges.

In the crystal, pairs of molecules are linked by pairwise N—H···N hydrogen bonds (Fig. 2; Table 1), forming inversion dimers with $R_2^2(16)$ ring motifs. C—H···O and C—H···π interactions (Table 1) further connect these dimers, constructing an extended three-dimensional structure.

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

*Cg*1, *Cg*3 and *Cg*4 are the centroids of the 4*H*-1,2,4-triazole ring (N2/C3/N3/N4/C4), the benzene ring (C12–C17) and the phenyl ring (C18–C23), respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N4^{i}	0.88	2.12	2.9949 (19)	177
C5—H5*B*···O4^{ii}	0.99	2.49	3.2838 (19)	137
C7—H7···O2^{i}	0.95	2.62	3.413 (2)	141
C19—H19···O3^{iii}	0.95	2.43	3.236 (2)	143
C23—H23···O2	0.95	2.55	3.194 (2)	125
C2—H2*A*···*Cg*4^{iv}	0.99	2.85	3.6592 (19)	140
C5—H5*B*···*Cg*1^{v}	0.99	2.92	3.433 (2)	113
C10—H10···*Cg*3^{vi}	0.95	2.67	3.5536 (18)	156
C14—H14···*Cg*1^{vii}	0.95	2.98	3.781 (2)	143

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

Synthesis and crystallization

A suspension of 5-(*p*-tolyloxy)methyl-4-phenyl-1,2,4- triazoline-3-thione (10 mmol), chloro-*N*-(*p*-nitrophenyl)- acetamide (10 mol) and anhydrous K_2CO_3 (2.0 g) in dry acetone (50 ml) was heated under reflux with stirring for 3 h. The hot reaction mixture was filtered to remove K_2CO_3 and the clear filtrate was evaporated to dryness. The solid residue was crystallized from ethanol solution to afford the title compound. Yield: 92%; m.p. 477 K. IR: 3240 (NH), 1670 (C═O) cm$^{-1.}$ ^{1}H NMR ($CDCl_3$): 9.4 (*s*, 1H, NH), 6.7–8.3 (*m*, 13H, ArH), 4.9 (*s*, 2H, OCH_2), 4.0 (*s*, 2H, SCH_2), 2.1 (*s*, 3H, CH_3) p.p.m..

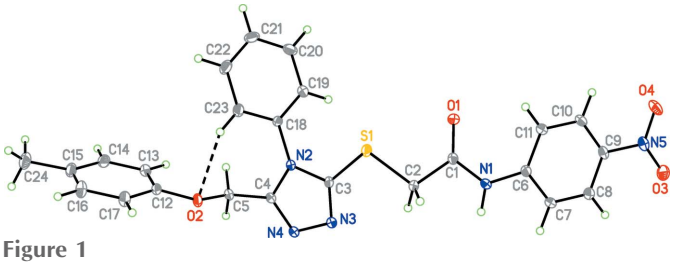


Figure 1
The molecular structure of the title molecule, shown with 50% probability displacement ellipsoids. The intramolecular hydrogen bond is shown as a dashed line.

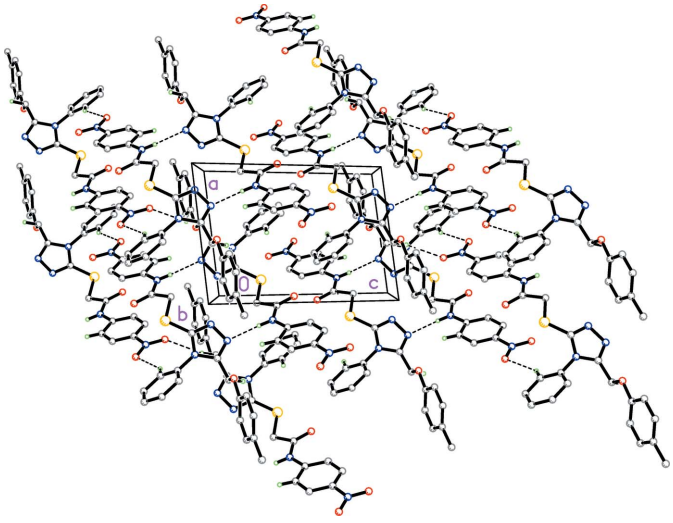


Figure 2
Packing of the title molecule viewed down the *b* axis, with hydrogen bonds shown as dashed lines.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{24}H_{21}N_5O_4S$
M_r	475.52
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	173
a, *b*, *c* (Å)	8.2241 (4), 12.2161 (7), 12.3952 (8)
α, β, γ (°)	115.507 (6), 93.532 (4), 96.914 (4)
V (Å^3)	1106.76 (12)
Z	2
Radiation type	Cu *Kα*
μ (mm^{-1})	1.67
Crystal size (mm)	0.06 × 0.06 × 0.04
Data collection	
Diffractometer	Rigaku Oxford Diffraction four-circle
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2014)
T_{min}, T_{max}	0.867, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7218, 4208, 3685
R_{int}	0.031
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.615
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.038, 0.102, 1.02
No. of reflections	4208
No. of parameters	308
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.27, −0.21

Computer programs: *CrysAlis PRO* (Agilent, 2014), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x161533 [https://doi.org/10.1107/S2414314616015339]

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Crystal data

$C_{24}H_{21}N_5O_4S$
M_r = 475.52
Triclinic, $P\overline{1}$
a = 8.2241 (4) Å
b = 12.2161 (7) Å
c = 12.3952 (8) Å
α = 115.507 (6)°
β = 93.532 (4)°
γ = 96.914 (4)°
V = 1106.76 (12) Å^3
Z = 2
$F(000)$ = 496
D_x = 1.427 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 3208 reflections
θ = 4.1–71.5°
μ = 1.67 mm^{-1}
T = 173 K
Prism, colourless
0.06 × 0.06 × 0.04 mm

Data collection

Rigaku Oxford Diffraction four-circle diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 16.0416 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2014)
T_{min} = 0.867, T_{max} = 1.000
7218 measured reflections
4208 independent reflections
3685 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 71.4°, θ_{min} = 4.0°
h = −9→8
k = −14→13
l = −11→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.102
S = 1.02
4208 reflections
308 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0525P)^2 + 0.2923P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.85636 (5)	0.52431 (4)	0.73550 (4)	0.02853 (13)
O1	0.97273 (15)	0.31095 (11)	0.56291 (10)	0.0278 (3)
O2	0.45307 (13)	0.80442 (10)	1.06977 (10)	0.0243 (2)
O3	1.43377 (17)	−0.21534 (12)	0.47098 (13)	0.0371 (3)
O4	1.30848 (18)	−0.22799 (12)	0.30651 (11)	0.0371 (3)
N1	1.14295 (17)	0.27467 (12)	0.69315 (12)	0.0232 (3)
H1	1.1841	0.3065	0.7696	0.028*
N2	0.60984 (16)	0.59879 (11)	0.87254 (11)	0.0193 (3)
N3	0.82466 (16)	0.57455 (12)	0.97176 (12)	0.0228 (3)
N4	0.70552 (17)	0.61560 (12)	1.04921 (12)	0.0226 (3)
N5	1.34846 (18)	−0.17518 (13)	0.41631 (13)	0.0268 (3)
C1	1.04125 (18)	0.34015 (14)	0.66351 (14)	0.0210 (3)
C2	1.0260 (2)	0.45989 (15)	0.77194 (14)	0.0256 (3)
H2A	1.1298	0.5190	0.7933	0.031*
H2B	1.0064	0.4437	0.8421	0.031*
C3	0.76396 (18)	0.56551 (13)	0.86744 (14)	0.0199 (3)
C4	0.58071 (18)	0.62961 (13)	0.98868 (14)	0.0197 (3)
C5	0.42806 (19)	0.67541 (14)	1.03736 (14)	0.0216 (3)
H5A	0.3307	0.6324	0.9756	0.026*
H5B	0.4098	0.6612	1.1088	0.026*
C6	1.19059 (19)	0.16297 (14)	0.61755 (14)	0.0210 (3)
C7	1.2798 (2)	0.10810 (15)	0.67497 (14)	0.0238 (3)
H7	1.3048	0.1475	0.7603	0.029*
C8	1.3318 (2)	−0.00215 (15)	0.60955 (15)	0.0248 (3)
H8	1.3929	−0.0390	0.6487	0.030*
C9	1.29292 (19)	−0.05829 (14)	0.48512 (14)	0.0234 (3)
C10	1.2067 (2)	−0.00546 (15)	0.42604 (14)	0.0254 (3)
H10	1.1828	−0.0453	0.3407	0.030*
C11	1.1553 (2)	0.10597 (15)	0.49199 (14)	0.0248 (3)
H11	1.0966	0.1433	0.4521	0.030*
C12	0.3168 (2)	0.86318 (15)	1.09212 (14)	0.0224 (3)
C13	0.1555 (2)	0.80569 (16)	1.07641 (15)	0.0258 (3)
H13	0.1309	0.7192	1.0488	0.031*
C14	0.0296 (2)	0.87682 (17)	1.10171 (16)	0.0297 (4)
H14	−0.0812	0.8372	1.0897	0.036*
C15	0.0612 (2)	1.00335 (17)	1.14384 (16)	0.0308 (4)
C16	0.2244 (2)	1.05886 (17)	1.15901 (18)	0.0351 (4)
H16	0.2492	1.1455	1.1877	0.042*
C17	0.3516 (2)	0.98984 (16)	1.13290 (17)	0.0303 (4)

H17	0.4621	1.0291	1.1429	0.036*
C18	0.49849 (18)	0.59151 (14)	0.77434 (13)	0.0192 (3)
C19	0.4528 (2)	0.47990 (15)	0.67390 (15)	0.0247 (3)
H19	0.4943	0.4089	0.6693	0.030*
C20	0.3451 (2)	0.47341 (18)	0.57963 (15)	0.0327 (4)
H20	0.3134	0.3976	0.5094	0.039*
C21	0.2835 (2)	0.5773 (2)	0.58765 (17)	0.0382 (4)
H21	0.2090	0.5723	0.5233	0.046*
C22	0.3302 (2)	0.68759 (19)	0.68882 (18)	0.0359 (4)
H22	0.2880	0.7584	0.6937	0.043*
C23	0.4384 (2)	0.69645 (15)	0.78381 (15)	0.0262 (3)
H23	0.4706	0.7725	0.8537	0.031*
C24	−0.0755 (3)	1.0801 (2)	1.1751 (2)	0.0413 (5)
H24A	−0.1814	1.0281	1.1327	0.062*
H24B	−0.0541	1.1463	1.1506	0.062*
H24C	−0.0797	1.1157	1.2622	0.062*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0298 (2)	0.0410 (2)	0.0215 (2)	0.02142 (17)	0.00957 (15)	0.01517 (18)
O1	0.0292 (6)	0.0312 (6)	0.0189 (6)	0.0121 (5)	−0.0009 (4)	0.0058 (5)
O2	0.0214 (5)	0.0185 (5)	0.0281 (6)	0.0071 (4)	0.0044 (4)	0.0047 (5)
O3	0.0416 (7)	0.0287 (7)	0.0399 (7)	0.0170 (5)	0.0058 (6)	0.0110 (6)
O4	0.0542 (8)	0.0279 (6)	0.0238 (7)	0.0121 (6)	0.0136 (6)	0.0039 (5)
N1	0.0269 (7)	0.0232 (7)	0.0152 (6)	0.0088 (5)	0.0011 (5)	0.0035 (5)
N2	0.0209 (6)	0.0185 (6)	0.0166 (6)	0.0079 (5)	0.0020 (5)	0.0049 (5)
N3	0.0226 (6)	0.0247 (7)	0.0183 (6)	0.0090 (5)	0.0019 (5)	0.0056 (5)
N4	0.0252 (7)	0.0224 (6)	0.0169 (6)	0.0087 (5)	0.0020 (5)	0.0045 (5)
N5	0.0291 (7)	0.0215 (7)	0.0277 (7)	0.0059 (5)	0.0105 (6)	0.0076 (6)
C1	0.0182 (7)	0.0231 (8)	0.0197 (7)	0.0059 (6)	0.0038 (5)	0.0067 (6)
C2	0.0224 (8)	0.0297 (8)	0.0207 (8)	0.0132 (6)	0.0013 (6)	0.0054 (7)
C3	0.0201 (7)	0.0179 (7)	0.0195 (7)	0.0076 (5)	0.0030 (5)	0.0051 (6)
C4	0.0219 (7)	0.0173 (7)	0.0167 (7)	0.0046 (5)	0.0015 (5)	0.0043 (6)
C5	0.0240 (8)	0.0186 (7)	0.0198 (7)	0.0076 (6)	0.0043 (6)	0.0051 (6)
C6	0.0205 (7)	0.0202 (7)	0.0194 (7)	0.0046 (5)	0.0031 (5)	0.0056 (6)
C7	0.0261 (8)	0.0261 (8)	0.0162 (7)	0.0065 (6)	0.0020 (6)	0.0061 (6)
C8	0.0261 (8)	0.0255 (8)	0.0236 (8)	0.0087 (6)	0.0042 (6)	0.0102 (7)
C9	0.0245 (8)	0.0192 (7)	0.0230 (8)	0.0050 (6)	0.0082 (6)	0.0052 (6)
C10	0.0295 (8)	0.0252 (8)	0.0161 (7)	0.0056 (6)	0.0043 (6)	0.0038 (6)
C11	0.0279 (8)	0.0267 (8)	0.0186 (8)	0.0086 (6)	0.0024 (6)	0.0079 (6)
C12	0.0240 (8)	0.0242 (8)	0.0196 (7)	0.0109 (6)	0.0051 (6)	0.0081 (6)
C13	0.0260 (8)	0.0263 (8)	0.0241 (8)	0.0075 (6)	0.0044 (6)	0.0091 (7)
C14	0.0249 (8)	0.0369 (9)	0.0295 (9)	0.0112 (7)	0.0064 (6)	0.0146 (8)
C15	0.0352 (9)	0.0346 (9)	0.0303 (9)	0.0193 (7)	0.0110 (7)	0.0170 (8)
C16	0.0390 (10)	0.0255 (9)	0.0448 (11)	0.0144 (7)	0.0116 (8)	0.0160 (8)
C17	0.0271 (8)	0.0247 (8)	0.0386 (10)	0.0071 (6)	0.0067 (7)	0.0123 (7)
C18	0.0174 (7)	0.0240 (7)	0.0175 (7)	0.0075 (5)	0.0031 (5)	0.0091 (6)

C19	0.0253 (8)	0.0249 (8)	0.0207 (8)	0.0073 (6)	0.0032 (6)	0.0064 (6)
C20	0.0266 (9)	0.0439 (10)	0.0188 (8)	0.0043 (7)	0.0009 (6)	0.0064 (7)
C21	0.0315 (9)	0.0656 (13)	0.0243 (9)	0.0183 (9)	0.0025 (7)	0.0237 (9)
C22	0.0393 (10)	0.0481 (11)	0.0353 (10)	0.0259 (8)	0.0113 (8)	0.0268 (9)
C23	0.0308 (8)	0.0258 (8)	0.0258 (8)	0.0123 (6)	0.0066 (6)	0.0125 (7)
C24	0.0420 (11)	0.0482 (12)	0.0473 (12)	0.0285 (9)	0.0189 (9)	0.0265 (10)

Geometric parameters (Å, º)

S1—C2	1.8062 (16)	C9—C10	1.381 (2)
S1—C3	1.7440 (15)	C10—H10	0.9500
O1—C1	1.217 (2)	C10—C11	1.387 (2)
O2—C5	1.4331 (19)	C11—H11	0.9500
O2—C12	1.3816 (19)	C12—C13	1.385 (2)
O3—N5	1.226 (2)	C12—C17	1.390 (2)
O4—N5	1.231 (2)	C13—H13	0.9500
N1—H1	0.8800	C13—C14	1.395 (2)
N1—C1	1.360 (2)	C14—H14	0.9500
N1—C6	1.402 (2)	C14—C15	1.386 (3)
N2—C3	1.3739 (19)	C15—C16	1.392 (3)
N2—C4	1.367 (2)	C15—C24	1.513 (2)
N2—C18	1.4415 (19)	C16—H16	0.9500
N3—N4	1.3973 (18)	C16—C17	1.389 (2)
N3—C3	1.311 (2)	C17—H17	0.9500
N4—C4	1.305 (2)	C18—C19	1.381 (2)
N5—C9	1.460 (2)	C18—C23	1.390 (2)
C1—C2	1.528 (2)	C19—H19	0.9500
C2—H2A	0.9900	C19—C20	1.390 (2)
C2—H2B	0.9900	C20—H20	0.9500
C4—C5	1.492 (2)	C20—C21	1.389 (3)
C5—H5A	0.9900	C21—H21	0.9500
C5—H5B	0.9900	C21—C22	1.377 (3)
C6—C7	1.400 (2)	C22—H22	0.9500
C6—C11	1.398 (2)	C22—C23	1.388 (3)
C7—H7	0.9500	C23—H23	0.9500
C7—C8	1.377 (2)	C24—H24A	0.9800
C8—H8	0.9500	C24—H24B	0.9800
C8—C9	1.388 (2)	C24—H24C	0.9800
C3—S1—C2	99.82 (8)	C9—C10—C11	119.64 (15)
C12—O2—C5	117.66 (12)	C11—C10—H10	120.2
C1—N1—H1	115.8	C6—C11—H11	120.3
C1—N1—C6	128.31 (14)	C10—C11—C6	119.48 (15)
C6—N1—H1	115.8	C10—C11—H11	120.3
C3—N2—C18	127.40 (13)	O2—C12—C13	125.17 (15)
C4—N2—C3	104.43 (12)	O2—C12—C17	114.73 (15)
C4—N2—C18	127.94 (13)	C13—C12—C17	120.10 (15)
C3—N3—N4	106.31 (12)	C12—C13—H13	120.5

C4—N4—N3	107.88 (12)	C12—C13—C14	118.91 (16)
O3—N5—O4	123.30 (14)	C14—C13—H13	120.5
O3—N5—C9	118.18 (14)	C13—C14—H14	118.9
O4—N5—C9	118.52 (15)	C15—C14—C13	122.12 (16)
O1—C1—N1	125.37 (14)	C15—C14—H14	118.9
O1—C1—C2	122.69 (14)	C14—C15—C16	117.81 (16)
N1—C1—C2	111.91 (13)	C14—C15—C24	121.68 (18)
S1—C2—H2A	109.8	C16—C15—C24	120.49 (17)
S1—C2—H2B	109.8	C15—C16—H16	119.4
C1—C2—S1	109.43 (11)	C17—C16—C15	121.14 (17)
C1—C2—H2A	109.8	C17—C16—H16	119.4
C1—C2—H2B	109.8	C12—C17—H17	120.0
H2A—C2—H2B	108.2	C16—C17—C12	119.90 (16)
N2—C3—S1	120.49 (11)	C16—C17—H17	120.0
N3—C3—S1	128.51 (12)	C19—C18—N2	119.01 (14)
N3—C3—N2	110.95 (13)	C19—C18—C23	121.77 (15)
N2—C4—C5	123.61 (14)	C23—C18—N2	119.21 (14)
N4—C4—N2	110.42 (13)	C18—C19—H19	120.6
N4—C4—C5	125.95 (14)	C18—C19—C20	118.73 (16)
O2—C5—C4	106.51 (12)	C20—C19—H19	120.6
O2—C5—H5A	110.4	C19—C20—H20	119.9
O2—C5—H5B	110.4	C21—C20—C19	120.28 (17)
C4—C5—H5A	110.4	C21—C20—H20	119.9
C4—C5—H5B	110.4	C20—C21—H21	120.0
H5A—C5—H5B	108.6	C22—C21—C20	120.01 (16)
C7—C6—N1	115.99 (14)	C22—C21—H21	120.0
C11—C6—N1	124.33 (15)	C21—C22—H22	119.6
C11—C6—C7	119.68 (15)	C21—C22—C23	120.73 (17)
C6—C7—H7	119.6	C23—C22—H22	119.6
C8—C7—C6	120.89 (15)	C18—C23—H23	120.8
C8—C7—H7	119.6	C22—C23—C18	118.46 (16)
C7—C8—H8	120.8	C22—C23—H23	120.8
C7—C8—C9	118.50 (15)	C15—C24—H24A	109.5
C9—C8—H8	120.8	C15—C24—H24B	109.5
C8—C9—N5	118.20 (15)	C15—C24—H24C	109.5
C10—C9—N5	119.99 (15)	H24A—C24—H24B	109.5
C10—C9—C8	121.80 (15)	H24A—C24—H24C	109.5
C9—C10—H10	120.2	H24B—C24—H24C	109.5

O1—C1—C2—S1	14.8 (2)	C4—N2—C18—C23	61.2 (2)
O2—C12—C13—C14	−179.47 (15)	C5—O2—C12—C13	−5.5 (2)
O2—C12—C17—C16	−179.65 (16)	C5—O2—C12—C17	174.82 (14)
O3—N5—C9—C8	−3.5 (2)	C6—N1—C1—O1	0.1 (3)
O3—N5—C9—C10	175.33 (15)	C6—N1—C1—C2	−177.91 (15)
O4—N5—C9—C8	176.98 (15)	C6—C7—C8—C9	−0.4 (2)
O4—N5—C9—C10	−4.2 (2)	C7—C6—C11—C10	1.1 (2)
N1—C1—C2—S1	−167.16 (11)	C7—C8—C9—N5	−179.99 (15)
N1—C6—C7—C8	179.55 (15)	C7—C8—C9—C10	1.2 (2)

N1—C6—C11—C10	−179.18 (15)	C8—C9—C10—C11	−0.8 (3)
N2—C4—C5—O2	−82.51 (17)	C9—C10—C11—C6	−0.4 (2)
N2—C18—C19—C20	179.83 (14)	C11—C6—C7—C8	−0.7 (2)
N2—C18—C23—C22	−179.48 (15)	C12—O2—C5—C4	165.95 (13)
N3—N4—C4—N2	0.43 (17)	C12—C13—C14—C15	−1.0 (3)
N3—N4—C4—C5	−178.18 (14)	C13—C12—C17—C16	0.6 (3)
N4—N3—C3—S1	177.46 (12)	C13—C14—C15—C16	0.9 (3)
N4—N3—C3—N2	0.00 (17)	C13—C14—C15—C24	−177.84 (17)
N4—C4—C5—O2	95.93 (18)	C14—C15—C16—C17	0.0 (3)
N5—C9—C10—C11	−179.59 (14)	C15—C16—C17—C12	−0.7 (3)
C1—N1—C6—C7	−172.03 (15)	C17—C12—C13—C14	0.2 (2)
C1—N1—C6—C11	8.3 (3)	C18—N2—C3—S1	7.8 (2)
C2—S1—C3—N2	−168.01 (12)	C18—N2—C3—N3	−174.54 (14)
C2—S1—C3—N3	14.74 (16)	C18—N2—C4—N4	174.33 (14)
C3—S1—C2—C1	135.78 (12)	C18—N2—C4—C5	−7.0 (2)
C3—N2—C4—N4	−0.42 (17)	C18—C19—C20—C21	−0.8 (3)
C3—N2—C4—C5	178.23 (14)	C19—C18—C23—C22	−0.3 (2)
C3—N2—C18—C19	55.5 (2)	C19—C20—C21—C22	0.6 (3)
C3—N2—C18—C23	−125.25 (17)	C20—C21—C22—C23	−0.2 (3)
C3—N3—N4—C4	−0.26 (17)	C21—C22—C23—C18	0.1 (3)
C4—N2—C3—S1	−177.45 (11)	C23—C18—C19—C20	0.6 (2)
C4—N2—C3—N3	0.25 (17)	C24—C15—C16—C17	178.74 (18)
C4—N2—C18—C19	−118.08 (17)		

Hydrogen-bond geometry (Å, º)

Cg1, Cg3 and Cg4 are the centroids of the 4*H*-1,2,4-triazole ring (N2/C3/N3/N4/C4), the benzene ring (C12–C17) and the phenyl ring (C18–C23), respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N4^{i}	0.88	2.12	2.9949 (19)	177
C5—H5*B*···O4^{ii}	0.99	2.49	3.2838 (19)	137
C7—H7···O2^{i}	0.95	2.62	3.413 (2)	141
C19—H19···O3^{iii}	0.95	2.43	3.236 (2)	143
C23—H23···O2	0.95	2.55	3.194 (2)	125
C2—H2*A*···*Cg*4^{iv}	0.99	2.85	3.6592 (19)	140
C5—H5*B*···*Cg*1^{v}	0.99	2.92	3.433 (2)	113
C10—H10···*Cg*3^{vi}	0.95	2.67	3.5536 (18)	156
C14—H14···*Cg*1^{vii}	0.95	2.98	3.781 (2)	143

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