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2-{[5-(4-Chlorophenoxymethyl)-4-phenyl-4*H*-1,2,4-triazol-3-yl]sulfanyl}-*N*-(4-nitrophenyl)acetamide

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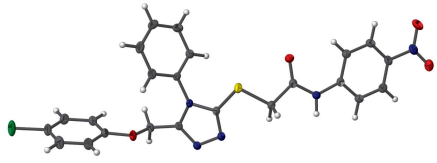
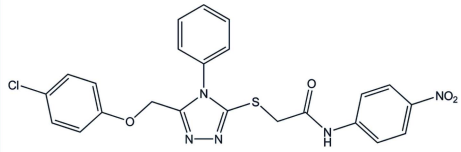
The title molecule, $C_{23}H_{18}ClN_5O_4S$, is in an 'extended' conformation. The central triazole ring makes dihedral angles of 58.14 (6), 86.29 (6) and 41.99 (6)°, respectively, with the adjacent phenyl, chlorophenyl and nitrophenyl rings. In the crystal, molecules are linked *via* a pair of N—H···N hydrogen bonds with an $R_2^2(16)$ ring motif, forming an inversion dimer. The dimers are connected by C—H···O hydrogen bonds into a tape structure along [011]. C—H···π interactions between the tapes are also observed.

3D view



Chemical scheme



Structure description

1,2,4-Triazole and its derivatives represent one of the most biologically active class of heterocyclic compounds. There are a large number of drugs containing a 1,2,4-triazole nucleus in their structures. These include Ribavirin (antiviral), Rizatriptan (anti-migraine), 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 infection diseases (Godhani *et al.*, 2015). In view of the above facts, we report in this context the synthesis and crystal structure of the title compound (Fig. 1).

In the crystal, molecules form a tape structure through N—H···N and C—H···O hydrogen bonds (Table 1 and Fig. 2). C—H···π interactions between the tapes contribute to the stabilization of the molecular packing.

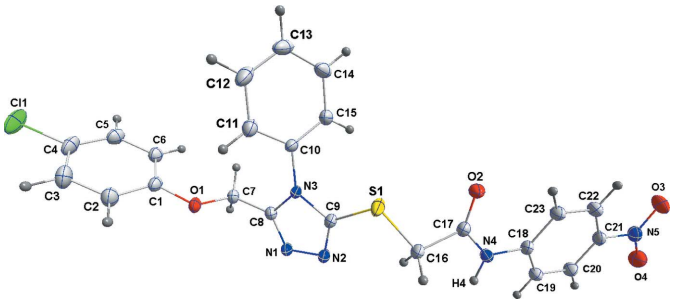


Figure 1
The molecular structure of the title compound, showing the atom-labeling scheme and 50% probability ellipsoids.

Synthesis and crystallization

A suspension of 5-(4-chlorphenoxy)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 until dryness. The solid residue was crystallized from ethanol to give the title compound. Yield: 93%; m.p. 207°C. IR (cm^{-1}): 3300 (NH), 1660 (C=O). ^{1}H NMR ($CDCl_3$, p.p.m.): δ 9.2 (*s*, 1H, NH), 6.7–8.0 (*m*, 13H, ArH), 4.9 (*s*, 2H, OCH_2), 4.0 (*s*, 2H,SCH_2).

Refinement

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

Acknowledgements

The support of NSF–MRI Grant No. 1228232 for the purchase of the diffractometer and Tulane University for support of the Tulane Crystallography Laboratory are gratefully acknowledged.

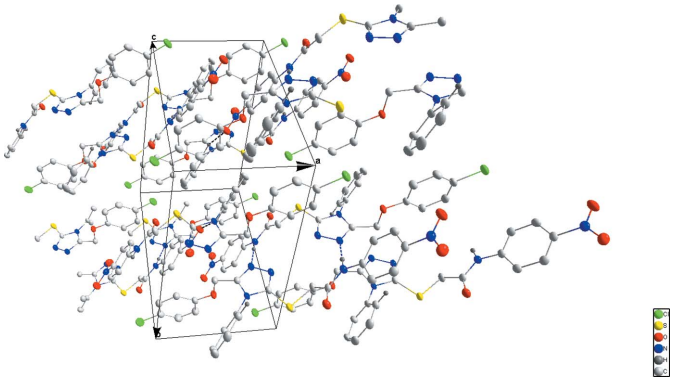


Figure 2
A packing diagram of the title compound, showing the tapes formed by N—H···N and C—H···O hydrogen bonds (blue and black dotted lines, respectively).

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

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the 1,2,4-triazole (N1/N2/C9/N3/C8), benzene (C1–C6) and phenyl (C10–C15) rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4···N1^{i}	0.91	2.08	2.9934 (17)	176
C15—H15···O4^{ii}	0.95	2.44	3.2324 (19)	140
C5—H5···*Cg*1^{iii}	0.95	2.97	3.757 (2)	141
C16—H16*A*···*Cg*3^{iv}	0.99	2.82	3.6284 (18)	139
C22—H22···*Cg*2^{v}	0.95	2.69	3.5883 (16)	158

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{23}H_{18}ClN_5O_4S$
M_r	495.93
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	150
a, *b*, *c* (Å)	8.1828 (2), 12.1541 (3), 12.3654 (3)
α, β, γ (°)	114.474 (1), 93.681 (1), 96.949 (1)
V (Å^3)	1102.14 (5)
Z	2
Radiation type	Cu *K*α
μ (mm^{-1})	2.79
Crystal size (mm)	0.21 × 0.18 × 0.03
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.80, 0.93
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8470, 4084, 3709
R_{int}	0.023
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.618
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.034, 0.089, 1.04
No. of reflections	4084
No. of parameters	307
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.17, −0.35

Computer programs: *APEX3* (Bruker, 2016), *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*b*), *SHELXL2014* (Sheldrick, 2015*a*), *DIAMOND* (Brandenburg & Putz, 2012).

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full crystallographic data

IUCrData (2016). **1**, x160452 [doi:10.1107/S2414314616004521]

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Crystal data

$C_{23}H_{18}ClN_5O_4S$
M_r = 495.93
Triclinic, $P\overline{1}$
a = 8.1828 (2) Å
b = 12.1541 (3) Å
c = 12.3654 (3) Å
α = 114.474 (1)°
β = 93.681 (1)°
γ = 96.949 (1)°
V = 1102.14 (5) Å^3
Z = 2
$F(000)$ = 512
D_x = 1.494 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 6886 reflections
θ = 4.0–72.3°
μ = 2.79 mm^{-1}
T = 150 K
Plate, colourless
0.21 × 0.18 × 0.03 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro–focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.80, T_{max} = 0.93
8470 measured reflections
4084 independent reflections
3709 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 72.3°, θ_{min} = 4.0°
h = −9→10
k = −14→13
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.089
S = 1.04
4084 reflections
307 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.048P)^2 + 0.4011P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	−0.09452 (6)	1.08937 (5)	1.17426 (5)	0.04449 (14)
S1	0.85499 (5)	0.52367 (4)	0.73580 (3)	0.02790 (12)
O1	0.45177 (13)	0.80389 (9)	1.06669 (9)	0.0230 (2)
O2	0.96933 (13)	0.31268 (10)	0.56493 (9)	0.0260 (2)
O3	1.30812 (16)	−0.22278 (10)	0.30629 (10)	0.0333 (3)
O4	1.43386 (15)	−0.21478 (10)	0.46972 (11)	0.0335 (3)
N1	0.70644 (15)	0.61703 (11)	1.04995 (11)	0.0215 (3)
N2	0.82617 (15)	0.57622 (11)	0.97273 (11)	0.0219 (3)
N3	0.60856 (14)	0.59829 (11)	0.87198 (10)	0.0184 (2)
N4	1.14142 (15)	0.27311 (11)	0.69377 (11)	0.0215 (3)
H4	1.1865	0.3031	0.7717	0.026*
N5	1.34798 (16)	−0.17258 (12)	0.41598 (12)	0.0253 (3)
C1	0.31563 (19)	0.86299 (14)	1.08991 (13)	0.0218 (3)
C2	0.3516 (2)	0.98921 (15)	1.13020 (15)	0.0289 (3)
H2	0.4630	1.0278	1.1399	0.035*
C3	0.2256 (2)	1.05892 (16)	1.15629 (16)	0.0335 (4)
H3	0.2500	1.1454	1.1848	0.040*
C4	0.0633 (2)	1.00125 (16)	1.14047 (15)	0.0300 (4)
C5	0.0266 (2)	0.87596 (16)	1.09983 (14)	0.0281 (3)
H5	−0.0854	0.8376	1.0887	0.034*
C6	0.15317 (19)	0.80536 (14)	1.07504 (13)	0.0241 (3)
H6	0.1287	0.7191	1.0484	0.029*
C7	0.42651 (18)	0.67518 (13)	1.03645 (13)	0.0208 (3)
H7A	0.3285	0.6324	0.9753	0.025*
H7B	0.4086	0.6607	1.1083	0.025*
C8	0.57961 (18)	0.63017 (12)	0.98852 (12)	0.0189 (3)
C9	0.76419 (17)	0.56569 (13)	0.86746 (13)	0.0197 (3)
C10	0.49571 (17)	0.58946 (13)	0.77336 (12)	0.0188 (3)
C11	0.4338 (2)	0.69254 (14)	0.77869 (14)	0.0255 (3)
H11	0.4648	0.7689	0.8467	0.031*
C12	0.3251 (2)	0.68181 (18)	0.68222 (15)	0.0344 (4)
H12	0.2811	0.7514	0.6844	0.041*
C13	0.2809 (2)	0.57079 (19)	0.58354 (15)	0.0354 (4)
H13	0.2066	0.5643	0.5181	0.043*
C14	0.3442 (2)	0.46872 (17)	0.57942 (14)	0.0299 (4)

H14	0.3138	0.3926	0.5109	0.036*
C15	0.45185 (19)	0.47706 (14)	0.67500 (13)	0.0230 (3)
H15	0.4946	0.4071	0.6730	0.028*
C16	1.02531 (19)	0.45839 (14)	0.77244 (13)	0.0244 (3)
H16A	1.1299	0.5171	0.7933	0.029*
H16B	1.0057	0.4410	0.8424	0.029*
C17	1.03937 (17)	0.34014 (13)	0.66470 (13)	0.0203 (3)
C18	1.18868 (18)	0.16229 (13)	0.61799 (13)	0.0202 (3)
C19	1.27723 (18)	0.10494 (14)	0.67439 (13)	0.0227 (3)
H19	1.3019	0.1421	0.7592	0.027*
C20	1.32914 (19)	−0.00431 (14)	0.60902 (13)	0.0237 (3)
H20	1.3893	−0.0429	0.6477	0.028*
C21	1.29176 (18)	−0.05704 (13)	0.48524 (13)	0.0222 (3)
C22	1.20524 (19)	−0.00199 (14)	0.42706 (13)	0.0232 (3)
H22	1.1816	−0.0396	0.3422	0.028*
C23	1.15320 (19)	0.10814 (14)	0.49296 (13)	0.0231 (3)
H23	1.0939	0.1466	0.4537	0.028*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0467 (3)	0.0525 (3)	0.0530 (3)	0.0368 (2)	0.0247 (2)	0.0304 (2)
S1	0.0279 (2)	0.0415 (2)	0.02153 (19)	0.02142 (17)	0.00882 (15)	0.01553 (16)
O1	0.0191 (5)	0.0182 (5)	0.0288 (5)	0.0078 (4)	0.0043 (4)	0.0056 (4)
O2	0.0258 (5)	0.0308 (6)	0.0187 (5)	0.0112 (5)	−0.0004 (4)	0.0067 (4)
O3	0.0445 (7)	0.0286 (6)	0.0223 (6)	0.0105 (5)	0.0096 (5)	0.0045 (5)
O4	0.0361 (6)	0.0279 (6)	0.0365 (6)	0.0152 (5)	0.0051 (5)	0.0111 (5)
N1	0.0220 (6)	0.0234 (6)	0.0170 (6)	0.0089 (5)	0.0021 (5)	0.0053 (5)
N2	0.0206 (6)	0.0253 (6)	0.0186 (6)	0.0098 (5)	0.0030 (5)	0.0063 (5)
N3	0.0177 (6)	0.0205 (6)	0.0169 (6)	0.0092 (5)	0.0023 (5)	0.0061 (4)
N4	0.0226 (6)	0.0235 (6)	0.0160 (6)	0.0089 (5)	0.0011 (5)	0.0049 (5)
N5	0.0260 (7)	0.0227 (6)	0.0256 (7)	0.0058 (5)	0.0083 (5)	0.0076 (5)
C1	0.0220 (7)	0.0243 (7)	0.0203 (7)	0.0107 (6)	0.0047 (6)	0.0085 (6)
C2	0.0275 (8)	0.0237 (8)	0.0349 (8)	0.0074 (7)	0.0060 (7)	0.0108 (6)
C3	0.0397 (9)	0.0246 (8)	0.0398 (9)	0.0144 (7)	0.0108 (8)	0.0138 (7)
C4	0.0320 (9)	0.0357 (9)	0.0312 (8)	0.0214 (7)	0.0122 (7)	0.0175 (7)
C5	0.0231 (7)	0.0354 (9)	0.0291 (8)	0.0102 (7)	0.0067 (6)	0.0151 (7)
C6	0.0238 (7)	0.0254 (7)	0.0235 (7)	0.0086 (6)	0.0055 (6)	0.0091 (6)
C7	0.0206 (7)	0.0190 (7)	0.0208 (7)	0.0064 (6)	0.0038 (6)	0.0055 (5)
C8	0.0205 (7)	0.0171 (6)	0.0173 (6)	0.0058 (6)	0.0025 (5)	0.0048 (5)
C9	0.0177 (7)	0.0201 (7)	0.0202 (7)	0.0077 (6)	0.0023 (5)	0.0064 (5)
C10	0.0164 (6)	0.0244 (7)	0.0174 (7)	0.0074 (6)	0.0021 (5)	0.0095 (5)
C11	0.0296 (8)	0.0262 (8)	0.0250 (7)	0.0129 (6)	0.0065 (6)	0.0125 (6)
C12	0.0390 (9)	0.0474 (10)	0.0313 (9)	0.0273 (8)	0.0115 (8)	0.0246 (8)
C13	0.0283 (8)	0.0634 (12)	0.0216 (8)	0.0206 (8)	0.0050 (7)	0.0211 (8)
C14	0.0237 (7)	0.0418 (9)	0.0187 (7)	0.0062 (7)	0.0020 (6)	0.0073 (6)
C15	0.0220 (7)	0.0252 (7)	0.0205 (7)	0.0077 (6)	0.0037 (6)	0.0074 (6)
C16	0.0206 (7)	0.0287 (8)	0.0201 (7)	0.0113 (6)	0.0014 (6)	0.0049 (6)

C17	0.0164 (6)	0.0237 (7)	0.0198 (7)	0.0055 (6)	0.0037 (5)	0.0076 (6)
C18	0.0174 (6)	0.0219 (7)	0.0199 (7)	0.0059 (6)	0.0037 (5)	0.0066 (6)
C19	0.0228 (7)	0.0260 (7)	0.0176 (7)	0.0063 (6)	0.0020 (6)	0.0072 (6)
C20	0.0234 (7)	0.0258 (7)	0.0237 (7)	0.0082 (6)	0.0029 (6)	0.0113 (6)
C21	0.0213 (7)	0.0210 (7)	0.0222 (7)	0.0058 (6)	0.0068 (6)	0.0061 (6)
C22	0.0243 (7)	0.0254 (7)	0.0172 (7)	0.0048 (6)	0.0028 (6)	0.0062 (6)
C23	0.0241 (7)	0.0261 (8)	0.0189 (7)	0.0081 (6)	0.0019 (6)	0.0084 (6)

Geometric parameters (Å, º)

Cl1—C4	1.7387 (16)	C7—C8	1.487 (2)
S1—C9	1.7383 (15)	C7—H7A	0.9900
S1—C16	1.8061 (15)	C7—H7B	0.9900
O1—C1	1.3796 (18)	C10—C11	1.386 (2)
O1—C7	1.4343 (18)	C10—C15	1.387 (2)
O2—C17	1.2181 (18)	C11—C12	1.392 (2)
O3—N5	1.2360 (17)	C11—H11	0.9500
O4—N5	1.2281 (18)	C12—C13	1.379 (3)
N1—C8	1.3111 (19)	C12—H12	0.9500
N1—N2	1.4010 (18)	C13—C14	1.384 (3)
N2—C9	1.3151 (18)	C13—H13	0.9500
N3—C8	1.3734 (19)	C14—C15	1.389 (2)
N3—C9	1.3765 (18)	C14—H14	0.9500
N3—C10	1.4403 (17)	C15—H15	0.9500
N4—C17	1.3634 (19)	C16—C17	1.525 (2)
N4—C18	1.4031 (18)	C16—H16A	0.9900
N4—H4	0.9098	C16—H16B	0.9900
N5—C21	1.4586 (19)	C18—C19	1.399 (2)
C1—C2	1.388 (2)	C18—C23	1.400 (2)
C1—C6	1.389 (2)	C19—C20	1.374 (2)
C2—C3	1.383 (2)	C19—H19	0.9500
C2—H2	0.9500	C20—C21	1.388 (2)
C3—C4	1.386 (3)	C20—H20	0.9500
C3—H3	0.9500	C21—C22	1.384 (2)
C4—C5	1.377 (2)	C22—C23	1.384 (2)
C5—C6	1.393 (2)	C22—H22	0.9500
C5—H5	0.9500	C23—H23	0.9500
C6—H6	0.9500		
C9—S1—C16	100.00 (7)	C11—C10—N3	119.63 (13)
C1—O1—C7	117.68 (12)	C15—C10—N3	118.71 (13)
C8—N1—N2	107.77 (12)	C10—C11—C12	118.59 (15)
C9—N2—N1	106.62 (11)	C10—C11—H11	120.7
C8—N3—C9	104.71 (11)	C12—C11—H11	120.7
C8—N3—C10	127.83 (12)	C13—C12—C11	120.44 (15)
C9—N3—C10	127.22 (12)	C13—C12—H12	119.8
C17—N4—C18	128.21 (12)	C11—C12—H12	119.8
C17—N4—H4	117.2	C12—C13—C14	120.28 (15)

C18—N4—H4	114.6	C12—C13—H13	119.9
O4—N5—O3	123.20 (13)	C14—C13—H13	119.9
O4—N5—C21	118.18 (13)	C13—C14—C15	120.28 (15)
O3—N5—C21	118.62 (13)	C13—C14—H14	119.9
O1—C1—C2	114.63 (14)	C15—C14—H14	119.9
O1—C1—C6	124.88 (14)	C10—C15—C14	118.74 (15)
C2—C1—C6	120.50 (14)	C10—C15—H15	120.6
C3—C2—C1	120.19 (16)	C14—C15—H15	120.6
C3—C2—H2	119.9	C17—C16—S1	109.03 (10)
C1—C2—H2	119.9	C17—C16—H16A	109.9
C2—C3—C4	119.29 (16)	S1—C16—H16A	109.9
C2—C3—H3	120.4	C17—C16—H16B	109.9
C4—C3—H3	120.4	S1—C16—H16B	109.9
C5—C4—C3	120.85 (15)	H16A—C16—H16B	108.3
C5—C4—Cl1	120.03 (14)	O2—C17—N4	125.33 (13)
C3—C4—Cl1	119.12 (13)	O2—C17—C16	122.69 (13)
C4—C5—C6	120.16 (15)	N4—C17—C16	111.96 (12)
C4—C5—H5	119.9	C19—C18—C23	119.61 (13)
C6—C5—H5	119.9	C19—C18—N4	116.02 (13)
C1—C6—C5	119.00 (15)	C23—C18—N4	124.37 (13)
C1—C6—H6	120.5	C20—C19—C18	121.02 (13)
C5—C6—H6	120.5	C20—C19—H19	119.5
O1—C7—C8	106.20 (12)	C18—C19—H19	119.5
O1—C7—H7A	110.5	C19—C20—C21	118.54 (14)
C8—C7—H7A	110.5	C19—C20—H20	120.7
O1—C7—H7B	110.5	C21—C20—H20	120.7
C8—C7—H7B	110.5	C22—C21—C20	121.67 (14)
H7A—C7—H7B	108.7	C22—C21—N5	119.88 (13)
N1—C8—N3	110.23 (13)	C20—C21—N5	118.45 (13)
N1—C8—C7	125.83 (13)	C21—C22—C23	119.76 (14)
N3—C8—C7	123.93 (12)	C21—C22—H22	120.1
N2—C9—N3	110.67 (13)	C23—C22—H22	120.1
N2—C9—S1	128.89 (11)	C22—C23—C18	119.40 (13)
N3—C9—S1	120.39 (10)	C22—C23—H23	120.3
C11—C10—C15	121.66 (13)	C18—C23—H23	120.3

C8—N1—N2—C9	−0.55 (16)	C8—N3—C10—C15	−118.65 (16)
C7—O1—C1—C2	173.83 (13)	C9—N3—C10—C15	54.9 (2)
C7—O1—C1—C6	−6.6 (2)	C15—C10—C11—C12	−0.1 (2)
O1—C1—C2—C3	179.81 (15)	N3—C10—C11—C12	179.91 (14)
C6—C1—C2—C3	0.2 (2)	C10—C11—C12—C13	−0.2 (3)
C1—C2—C3—C4	−0.7 (3)	C11—C12—C13—C14	0.0 (3)
C2—C3—C4—C5	0.3 (3)	C12—C13—C14—C15	0.5 (3)
C2—C3—C4—Cl1	179.61 (13)	C11—C10—C15—C14	0.6 (2)
C3—C4—C5—C6	0.6 (3)	N3—C10—C15—C14	−179.44 (13)
Cl1—C4—C5—C6	−178.67 (12)	C13—C14—C15—C10	−0.7 (2)
O1—C1—C6—C5	−178.85 (14)	C9—S1—C16—C17	136.78 (11)
C2—C1—C6—C5	0.7 (2)	C18—N4—C17—O2	0.8 (3)

C4—C5—C6—C1	−1.1 (2)	C18—N4—C17—C16	−177.53 (14)
C1—O1—C7—C8	166.87 (12)	S1—C16—C17—O2	14.43 (19)
N2—N1—C8—N3	0.69 (16)	S1—C16—C17—N4	−167.17 (11)
N2—N1—C8—C7	−178.20 (13)	C17—N4—C18—C19	−171.74 (14)
C9—N3—C8—N1	−0.55 (16)	C17—N4—C18—C23	8.4 (2)
C10—N3—C8—N1	174.12 (13)	C23—C18—C19—C20	−0.4 (2)
C9—N3—C8—C7	178.37 (13)	N4—C18—C19—C20	179.69 (14)
C10—N3—C8—C7	−7.0 (2)	C18—C19—C20—C21	0.0 (2)
O1—C7—C8—N1	95.45 (17)	C19—C20—C21—C22	0.4 (2)
O1—C7—C8—N3	−83.30 (16)	C19—C20—C21—N5	179.58 (14)
N1—N2—C9—N3	0.21 (16)	O4—N5—C21—C22	175.23 (14)
N1—N2—C9—S1	177.76 (11)	O3—N5—C21—C22	−4.3 (2)
C8—N3—C9—N2	0.19 (16)	O4—N5—C21—C20	−3.9 (2)
C10—N3—C9—N2	−174.52 (13)	O3—N5—C21—C20	176.57 (14)
C8—N3—C9—S1	−177.60 (10)	C20—C21—C22—C23	−0.3 (2)
C10—N3—C9—S1	7.7 (2)	N5—C21—C22—C23	−179.48 (14)
C16—S1—C9—N2	15.55 (16)	C21—C22—C23—C18	−0.1 (2)
C16—S1—C9—N3	−167.10 (12)	C19—C18—C23—C22	0.5 (2)
C8—N3—C10—C11	61.4 (2)	N4—C18—C23—C22	−179.62 (14)
C9—N3—C10—C11	−125.12 (16)		

Hydrogen-bond geometry (Å, º)

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the 1,2,4-triazole (N1/N2/C9/N3/C8), benzene (C1–C6) and phenyl (C10–C15) rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4···N1^{i}	0.91	2.08	2.9934 (17)	176
C15—H15···O4^{ii}	0.95	2.44	3.2324 (19)	140
C5—H5···*Cg*1^{iii}	0.95	2.97	3.757 (2)	141
C16—H16*A*···*Cg*3^{iv}	0.99	2.82	3.6284 (18)	139
C22—H22···*Cg*2^{v}	0.95	2.69	3.5883 (16)	158

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