2-({5-[(4-Chlorophenoxy)methyl]-4-phenyl-4*H*-1,2,4-triazol-3-yl}sulfanyl)-*N*-phenylacetamide

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The title molecule, $C_{23}H_{19}ClN_4O_2S$, is in an 'extended' conformation. In the crystal, pairwise N—H⋯N and C—H⋯O hydrogen bonds lead to the formation of 'stair-step' chains. C—H⋯π interactions further contribute to the consolidation of the molecular packing. The 4-chlorophenyl group is disordered over two sets of sites in a 0.948 (2):0.052 (2) ratio. The dihedral angle between the two components of the disordered chloro-substituted benzene ring is 15.76 (9) °.

3D view
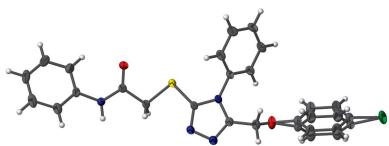
Chemical scheme
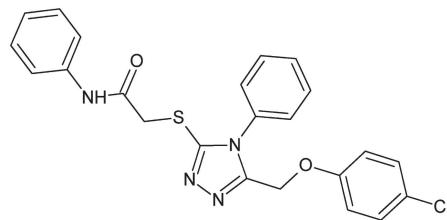
Structure description

In the last few years, the chemistry of 1,2,4-triazoles has received considerable attention owing to their synthetic and effective biological importance (Shaker, 2006). Many triazole compounds exhibited different biological properties such as antifungal, antibacterial, anti-inflammatory, ant-cancer, anti-malarial and analgesic activity (Bektaş *et al.*, 2010; Jawad *et al.*, 2012; Singhal *et al.*, 2011).

In the solid state, the molecule of the title compound (Fig. 1) is in an 'extended' conformation. The 1,2,4-triazole ring (N1–N3/C8/C9) forms dihedral angles of 62.57 (8) and 33.48 (8)°, with the phenyl ring (C10–C15) attached to the 1,2,4-triazol ring and the phenyl ring (C18–C23) of the *N*-phenylacetamide group, respectively. The dihedral angle between the two components of the disordered chloro-substituted benzene ring is 15.76 (9)°.

In the crystal, pairwise N4—H4⋯N1[i] [symmetry code: (i) −x + 1, −y + 1, −z + 1] hydrogen bonds form dimers, which are then associated into 'stair-step' chains through
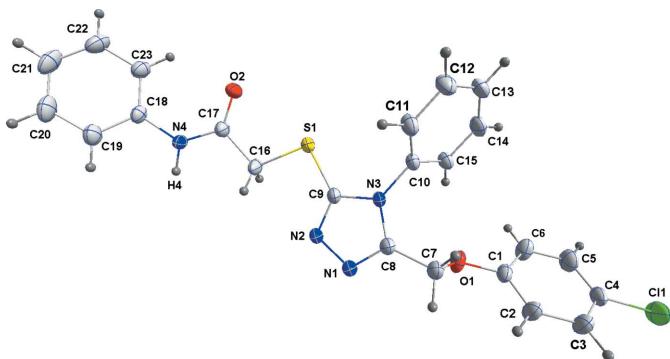
Figure 1
The molecular structure of the title compound with 50% probability ellipsoids.

pairwise C7—H7B···O2^{ii} [symmetry code: (ii) $x + \frac{1}{2}$, $y - \frac{1}{2}$, z] hydrogen bonds (Table 1 and Fig. 2). In addition, C—H···π interactions are observed in the crystal structure (Table 1).

Synthesis and crystallization

A suspension of 5-(4-chlorphenoxy)methyl-4-phenyl-1,2,4-triazoline-3-thione (10 mmol), chloro(N-phenyl)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 till dryness. The solid residue was crystallized from ethanol to give the title compound. Yield: 80%; m.p. 463 K. IR: 3300 (NH), 1670 (C=O) cm.$^{-1}$ ^{1}H NMR (DMSO-d_6): δ = 8.8 (s, 1H, NH), 6.5–7.8 (m, 14H, ArH), 4.9 (s, 2H, OCH$_2$), 3.9 (s, 2H,SCH$_2$).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The 4-chlorophenyl group is disordered over two orientations in a 0.948 (2): 0.052 (2) ratio. The minor component was refined as a rigid hexagon.
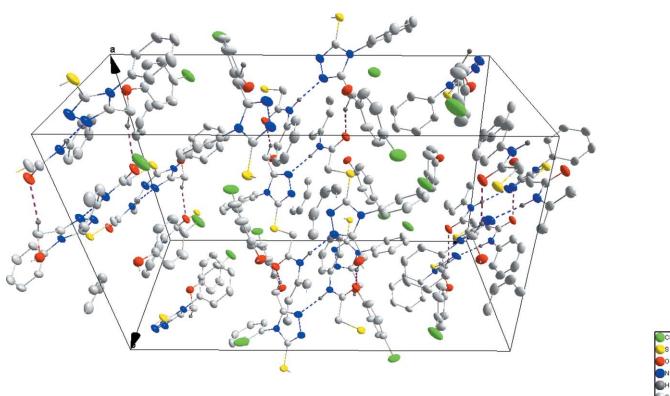

Figure 2
Packing projected onto (110). N—H···N and C—H···O hydrogen bonds are shown, respectively, as blue and purple dotted lines. Displacement ellipsoids are drawn at the 50% probability level.

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

Cg3 and Cg4 are the centroids of the C10–C15 and C18–C23 phenyl rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4···N1^i	0.91	2.02	2.9230 (17)	174
C7—H7B···O2^{ii}	0.99	2.49	3.3518 (18)	146
C3—H3···Cg3^{iii}	0.95	2.92	3.867 (2)	174
C15—H15···Cg4^{iv}	0.95	2.86	3.6871 (16)	146
C16—H16A···Cg4^v	0.99	2.80	3.6488 (18)	144

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

Table 2
Experimental details.

Crystal data	
Chemical formula	C$_{23}$H$_{19}$ClN$_4$O$_2$S
M_r	450.93
Crystal system, space group	Monoclinic, $C2/c$
Temperature (K)	150
a, b, c (Å)	15.7940 (12), 11.1864 (8), 24.8212 (18)
β (°)	95.128 (1)
V (Å^3)	4367.8 (6)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.30
Crystal size (mm)	0.24 × 0.20 × 0.11
Data collection	
Diffractometer	Bruker *SMART APEX* CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.86, 0.97
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	41579, 5886, 4471
R_{int}	0.045
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.686
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.043, 0.118, 1.06
No. of reflections	5886
No. of parameters	287
No. of restraints	2
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.41, −0.22

Computer programs: *APEX3* (Bruker, 2016), *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015a), *SHELXL2014* (Sheldrick, 2015b), *DIAMOND* (Brandenburg & Putz, 2012), *SHELXTL* (Sheldrick, 2008).

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full crystallographic data

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2-({5-[(4-Chlorophenoxy)methyl]-4-phenyl-4*H*-1,2,4-triazol-3-yl}sulfanyl)-*N*-phenylacetamide

Crystal data

$C_{23}H_{19}ClN_4O_2S$	$F(000) = 1872$
$M_r = 450.93$	$D_x = 1.371$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 15.7940$ (12) Å	Cell parameters from 9935 reflections
$b = 11.1864$ (8) Å	$\theta = 2.3$–28.9°
$c = 24.8212$ (18) Å	$\mu = 0.30$ mm^{-1}
$\beta = 95.128$ (1)°	$T = 150$ K
$V = 4367.8$ (6) Å^3	Block, colourless
$Z = 8$	$0.24 \times 0.20 \times 0.11$ mm

Data collection

Bruker SMART APEX CCD diffractometer	41579 measured reflections
Radiation source: fine-focus sealed tube	5886 independent reflections
Graphite monochromator	4471 reflections with $I > 2\sigma(I)$
Detector resolution: 8.3333 pixels mm^{-1}	$R_{int} = 0.045$
φ and ω scans	$\theta_{max} = 29.2°$, $\theta_{min} = 1.7°$
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)	$h = -21 \rightarrow 21$
	$k = -14 \rightarrow 15$
$T_{min} = 0.86$, $T_{max} = 0.97$	$l = -33 \rightarrow 34$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.043$	Hydrogen site location: mixed
$wR(F^2) = 0.118$	H-atom parameters constrained
$S = 1.06$	$w = 1/[\sigma^2(F_o^2) + (0.0604P)^2 + 1.3119P]$
5886 reflections	where $P = (F_o^2 + 2F_c^2)/3$
287 parameters	$(\Delta/\sigma)_{max} < 0.001$
2 restraints	$\Delta\rho_{max} = 0.41$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{min} = -0.21$ e Å^{-3}

Special details

Experimental. The diffraction data were obtained from 3 sets of 400 frames, each of width 0.5° in ω, colllected at φ = 0.00, 90.00 and 180.00° and 2 sets of 800 frames, each of width 0.45° in φ, collected at $\omega = -30.00$ and 210.00°. The scan time was 20 sec/frame.

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. H-atoms attached to carbon were placed in calculated positions (C—H = 0.95 − 0.99 Å) while that attached to nitrogen was placed in a location derived from a difference map and its coordinates adjusted to give N—H = 0.91%A. All were included as riding contributions with isotropic displacement parameters 1.2 times those of the attached atoms. The 4-chlorophenyl group is disordered over two orientations in a 95:5 ratio. The minor component was refined as a rigid hexagon.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Cl1	0.58100 (3)	−0.46695 (4)	0.30292 (2)	0.06539 (18)	
S1	0.33857 (2)	0.45849 (3)	0.39103 (2)	0.02814 (10)	
O1	0.50609 (7)	0.00496 (9)	0.38890 (4)	0.0346 (2)	
O2	0.26017 (7)	0.68130 (9)	0.39453 (4)	0.0356 (3)	
N1	0.53671 (8)	0.27205 (11)	0.44169 (5)	0.0323 (3)	
N2	0.48065 (8)	0.36629 (11)	0.44741 (5)	0.0298 (3)	
N3	0.43815 (7)	0.26509 (9)	0.37347 (4)	0.0226 (2)	
N4	0.33954 (7)	0.76835 (10)	0.46533 (5)	0.0257 (2)	
H4	0.3802	0.7527	0.4927	0.031*	
C1	0.52663 (12)	−0.10073 (13)	0.36507 (7)	0.0287 (4)	0.948 (2)
C2	0.60655 (11)	−0.12626 (15)	0.35021 (8)	0.0393 (4)	0.948 (2)
H2	0.6499	−0.0672	0.3536	0.047*	0.948 (2)
C3	0.62341 (12)	−0.23890 (16)	0.33017 (8)	0.0452 (5)	0.948 (2)
H3	0.6786	−0.2580	0.3204	0.054*	0.948 (2)
C4	0.55925 (12)	−0.32265 (15)	0.32458 (7)	0.0379 (4)	0.948 (2)
C5	0.47874 (12)	−0.29637 (15)	0.33764 (8)	0.0410 (4)	0.948 (2)
H5	0.4349	−0.3545	0.3328	0.049*	0.948 (2)
C6	0.46197 (11)	−0.18450 (15)	0.35786 (7)	0.0383 (4)	0.948 (2)
H6	0.4063	−0.1651	0.3668	0.046*	0.948 (2)
C1A	0.5373 (18)	−0.1082 (12)	0.3766 (10)	0.0287 (4)	0.052 (2)
C2A	0.5741 (17)	−0.1263 (15)	0.3285 (9)	0.0393 (4)	0.052 (2)
H2A	0.5901	−0.0597	0.3079	0.047*	0.052 (2)
C3A	0.5875 (17)	−0.2418 (19)	0.3104 (8)	0.0452 (5)	0.052 (2)
H3A	0.6126	−0.2542	0.2775	0.054*	0.052 (2)
C4A	0.5641 (19)	−0.3392 (13)	0.3406 (9)	0.0379 (4)	0.052 (2)
C5A	0.5273 (16)	−0.3211 (13)	0.3887 (9)	0.0410 (4)	0.052 (2)
H5A	0.5113	−0.3877	0.4093	0.049*	0.052 (2)
C6A	0.5139 (15)	−0.2056 (16)	0.4068 (8)	0.0383 (4)	0.052 (2)
H6A	0.4887	−0.1932	0.4397	0.046*	0.052 (2)
C7	0.55380 (9)	0.10811 (12)	0.37635 (6)	0.0300 (3)	
H7A	0.5558	0.1153	0.3367	0.036*	
H7B	0.6128	0.1021	0.3934	0.036*	
C8	0.51050 (9)	0.21362 (12)	0.39776 (6)	0.0262 (3)	

C9	0.42313 (8)	0.36036 (11)	0.40612 (5)	0.0238 (3)
C10	0.38827 (8)	0.22517 (12)	0.32540 (5)	0.0226 (3)
C11	0.37983 (10)	0.29843 (13)	0.28040 (6)	0.0327 (3)
H11	0.4063	0.3747	0.2811	0.039*
C12	0.33191 (11)	0.25847 (14)	0.23410 (6)	0.0386 (4)
H12	0.3247	0.3085	0.2031	0.046*
C13	0.29497 (10)	0.14698 (14)	0.23290 (6)	0.0349 (3)
H13	0.2630	0.1199	0.2010	0.042*
C14	0.30446 (10)	0.07439 (14)	0.27815 (6)	0.0339 (3)
H14	0.2793	−0.0028	0.2771	0.041*
C15	0.35049 (9)	0.11348 (12)	0.32500 (6)	0.0269 (3)
H15	0.3560	0.0644	0.3563	0.032*
C16	0.36384 (11)	0.56155 (13)	0.44629 (6)	0.0328 (3)
H16A	0.3468	0.5275	0.4805	0.039*
H16B	0.4257	0.5776	0.4506	0.039*
C17	0.31512 (9)	0.67619 (12)	0.43258 (5)	0.0260 (3)
C18	0.31242 (9)	0.88903 (12)	0.46004 (5)	0.0253 (3)
C19	0.36564 (11)	0.97533 (13)	0.48553 (6)	0.0340 (3)
H19	0.4176	0.9520	0.5050	0.041*
C20	0.34301 (13)	1.09500 (14)	0.48259 (7)	0.0426 (4)
H20	0.3795	1.1534	0.5001	0.051*
C21	0.26751 (13)	1.12977 (14)	0.45431 (7)	0.0441 (4)
H21	0.2521	1.2118	0.4522	0.053*
C22	0.21490 (12)	1.04423 (14)	0.42929 (7)	0.0413 (4)
H22	0.1628	1.0680	0.4102	0.050*
C23	0.23653 (10)	0.92380 (14)	0.43150 (6)	0.0326 (3)
H23	0.2000	0.8659	0.4137	0.039*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0626 (3)	0.0424 (3)	0.0857 (4)	0.0196 (2)	−0.0237 (3)	−0.0402 (3)
S1	0.02955 (18)	0.02184 (18)	0.0311 (2)	0.00325 (13)	−0.00802 (14)	−0.00773 (13)
O1	0.0408 (6)	0.0215 (5)	0.0433 (6)	0.0016 (4)	0.0128 (5)	−0.0058 (4)
O2	0.0428 (6)	0.0307 (6)	0.0301 (6)	0.0088 (5)	−0.0134 (5)	−0.0077 (4)
N1	0.0330 (6)	0.0258 (6)	0.0359 (7)	0.0051 (5)	−0.0098 (5)	−0.0085 (5)
N2	0.0341 (6)	0.0230 (6)	0.0303 (6)	0.0038 (5)	−0.0086 (5)	−0.0072 (5)
N3	0.0261 (5)	0.0176 (5)	0.0233 (6)	−0.0010 (4)	−0.0026 (4)	−0.0039 (4)
N4	0.0307 (6)	0.0210 (6)	0.0242 (6)	0.0047 (4)	−0.0045 (5)	−0.0031 (4)
C1	0.0375 (9)	0.0215 (7)	0.0267 (9)	0.0059 (6)	0.0009 (7)	−0.0028 (6)
C2	0.0271 (8)	0.0300 (8)	0.0598 (12)	0.0046 (6)	−0.0020 (8)	−0.0135 (8)
C3	0.0313 (9)	0.0409 (10)	0.0618 (13)	0.0121 (8)	−0.0047 (9)	−0.0187 (9)
C4	0.0446 (9)	0.0289 (9)	0.0373 (10)	0.0125 (7)	−0.0117 (8)	−0.0140 (7)
C5	0.0467 (10)	0.0269 (8)	0.0496 (10)	−0.0044 (7)	0.0051 (8)	−0.0071 (7)
C6	0.0394 (9)	0.0290 (8)	0.0482 (10)	0.0002 (7)	0.0137 (8)	−0.0044 (7)
C1A	0.0375 (9)	0.0215 (7)	0.0267 (9)	0.0059 (6)	0.0009 (7)	−0.0028 (6)
C2A	0.0271 (8)	0.0300 (8)	0.0598 (12)	0.0046 (6)	−0.0020 (8)	−0.0135 (8)
C3A	0.0313 (9)	0.0409 (10)	0.0618 (13)	0.0121 (8)	−0.0047 (9)	−0.0187 (9)

C4A	0.0446 (9)	0.0289 (9)	0.0373 (10)	0.0125 (7)	−0.0117 (8)	−0.0140 (7)
C5A	0.0467 (10)	0.0269 (8)	0.0496 (10)	−0.0044 (7)	0.0051 (8)	−0.0071 (7)
C6A	0.0394 (9)	0.0290 (8)	0.0482 (10)	0.0002 (7)	0.0137 (8)	−0.0044 (7)
C7	0.0275 (7)	0.0239 (7)	0.0380 (8)	0.0010 (5)	−0.0008 (6)	−0.0060 (6)
C8	0.0264 (6)	0.0218 (7)	0.0294 (7)	0.0005 (5)	−0.0028 (5)	−0.0029 (5)
C9	0.0275 (6)	0.0187 (6)	0.0245 (7)	−0.0005 (5)	−0.0022 (5)	−0.0038 (5)
C10	0.0256 (6)	0.0208 (6)	0.0210 (6)	−0.0012 (5)	0.0006 (5)	−0.0057 (5)
C11	0.0475 (9)	0.0235 (7)	0.0265 (7)	−0.0070 (6)	−0.0006 (6)	−0.0020 (6)
C12	0.0575 (10)	0.0342 (8)	0.0227 (7)	−0.0004 (7)	−0.0044 (7)	0.0004 (6)
C13	0.0389 (8)	0.0392 (8)	0.0253 (7)	0.0004 (6)	−0.0047 (6)	−0.0114 (6)
C14	0.0362 (8)	0.0295 (7)	0.0350 (8)	−0.0081 (6)	−0.0015 (6)	−0.0098 (6)
C15	0.0313 (7)	0.0239 (7)	0.0251 (7)	−0.0050 (5)	0.0006 (6)	−0.0026 (5)
C16	0.0482 (9)	0.0246 (7)	0.0237 (7)	0.0112 (6)	−0.0077 (6)	−0.0076 (5)
C17	0.0324 (7)	0.0235 (7)	0.0216 (6)	0.0036 (5)	−0.0003 (5)	−0.0029 (5)
C18	0.0346 (7)	0.0204 (6)	0.0214 (6)	0.0029 (5)	0.0053 (5)	−0.0020 (5)
C19	0.0411 (8)	0.0271 (8)	0.0341 (8)	−0.0014 (6)	0.0042 (7)	−0.0052 (6)
C20	0.0661 (11)	0.0245 (8)	0.0388 (9)	−0.0061 (7)	0.0130 (8)	−0.0062 (7)
C21	0.0768 (13)	0.0228 (8)	0.0344 (9)	0.0115 (8)	0.0142 (8)	0.0005 (6)
C22	0.0579 (10)	0.0332 (9)	0.0328 (8)	0.0173 (7)	0.0041 (8)	0.0045 (7)
C23	0.0418 (8)	0.0277 (7)	0.0279 (7)	0.0078 (6)	0.0004 (6)	−0.0007 (6)

Geometric parameters (Å, º)

Cl1—C4A	1.741 (11)	C4A—C5A	1.3900
Cl1—C4	1.7452 (16)	C5A—C6A	1.3900
S1—C9	1.7434 (14)	C5A—H5A	0.9500
S1—C16	1.8089 (14)	C6A—H6A	0.9500
O1—C1	1.3738 (17)	C7—C8	1.4861 (19)
O1—C1A	1.402 (11)	C7—H7A	0.9900
O1—C7	1.4277 (18)	C7—H7B	0.9900
O2—C17	1.2257 (17)	C10—C11	1.3822 (19)
N1—C8	1.3065 (18)	C10—C15	1.3843 (18)
N1—N2	1.3920 (16)	C11—C12	1.392 (2)
N2—C9	1.3092 (17)	C11—H11	0.9500
N3—C8	1.3703 (17)	C12—C13	1.376 (2)
N3—C9	1.3724 (16)	C12—H12	0.9500
N3—C10	1.4405 (16)	C13—C14	1.383 (2)
N4—C17	1.3477 (17)	C13—H13	0.9500
N4—C18	1.4189 (17)	C14—C15	1.3858 (19)
N4—H4	0.9098	C14—H14	0.9500
C1—C2	1.376 (2)	C15—H15	0.9500
C1—C6	1.386 (2)	C16—C17	1.5184 (19)
C2—C3	1.389 (2)	C16—H16A	0.9900
C2—H2	0.9500	C16—H16B	0.9900
C3—C4	1.378 (3)	C18—C23	1.392 (2)
C3—H3	0.9500	C18—C19	1.394 (2)
C4—C5	1.372 (3)	C19—C20	1.386 (2)
C5—C6	1.383 (2)	C19—H19	0.9500

C5—H5	0.9500	C20—C21	1.384 (3)
C6—H6	0.9500	C20—H20	0.9500
C1A—C2A	1.3900	C21—C22	1.378 (3)
C1A—C6A	1.3900	C21—H21	0.9500
C2A—C3A	1.3900	C22—C23	1.390 (2)
C2A—H2A	0.9500	C22—H22	0.9500
C3A—C4A	1.3900	C23—H23	0.9500
C3A—H3A	0.9500		
C9—S1—C16	97.21 (6)	H7A—C7—H7B	108.5
C1—O1—C7	116.88 (12)	N1—C8—N3	110.29 (12)
C1A—O1—C7	118.7 (10)	N1—C8—C7	125.05 (13)
C8—N1—N2	107.88 (11)	N3—C8—C7	124.65 (12)
C9—N2—N1	106.56 (11)	N2—C9—N3	110.93 (12)
C8—N3—C9	104.34 (11)	N2—C9—S1	126.94 (10)
C8—N3—C10	127.37 (11)	N3—C9—S1	122.12 (10)
C9—N3—C10	128.26 (11)	C11—C10—C15	121.26 (12)
C17—N4—C18	127.18 (12)	C11—C10—N3	119.45 (12)
C17—N4—H4	116.6	C15—C10—N3	119.29 (12)
C18—N4—H4	116.1	C10—C11—C12	118.87 (13)
O1—C1—C2	123.47 (16)	C10—C11—H11	120.6
O1—C1—C6	115.96 (15)	C12—C11—H11	120.6
C2—C1—C6	120.54 (14)	C13—C12—C11	120.47 (14)
C1—C2—C3	119.60 (17)	C13—C12—H12	119.8
C1—C2—H2	120.2	C11—C12—H12	119.8
C3—C2—H2	120.2	C12—C13—C14	119.96 (14)
C4—C3—C2	119.34 (16)	C12—C13—H13	120.0
C4—C3—H3	120.3	C14—C13—H13	120.0
C2—C3—H3	120.3	C13—C14—C15	120.45 (14)
C5—C4—C3	121.28 (15)	C13—C14—H14	119.8
C5—C4—Cl1	118.89 (15)	C15—C14—H14	119.8
C3—C4—Cl1	119.78 (14)	C10—C15—C14	118.97 (13)
C4—C5—C6	119.43 (16)	C10—C15—H15	120.5
C4—C5—H5	120.3	C14—C15—H15	120.5
C6—C5—H5	120.3	C17—C16—S1	107.17 (10)
C5—C6—C1	119.73 (16)	C17—C16—H16A	110.3
C5—C6—H6	120.1	S1—C16—H16A	110.3
C1—C6—H6	120.1	C17—C16—H16B	110.3
C2A—C1A—C6A	120.0	S1—C16—H16B	110.3
C2A—C1A—O1	120.0 (14)	H16A—C16—H16B	108.5
C6A—C1A—O1	118.4 (14)	O2—C17—N4	125.02 (12)
C1A—C2A—C3A	120.0	O2—C17—C16	121.46 (12)
C1A—C2A—H2A	120.0	N4—C17—C16	113.51 (12)
C3A—C2A—H2A	120.0	C23—C18—C19	119.62 (13)
C2A—C3A—C4A	120.0	C23—C18—N4	123.51 (13)
C2A—C3A—H3A	120.0	C19—C18—N4	116.87 (13)
C4A—C3A—H3A	120.0	C20—C19—C18	120.19 (15)
C3A—C4A—C5A	120.0	C20—C19—H19	119.9

C3A—C4A—Cl1	107.1 (13)	C18—C19—H19	119.9
C5A—C4A—Cl1	132.6 (13)	C21—C20—C19	120.30 (16)
C6A—C5A—C4A	120.0	C21—C20—H20	119.9
C6A—C5A—H5A	120.0	C19—C20—H20	119.9
C4A—C5A—H5A	120.0	C22—C21—C20	119.39 (15)
C5A—C6A—C1A	120.0	C22—C21—H21	120.3
C5A—C6A—H6A	120.0	C20—C21—H21	120.3
C1A—C6A—H6A	120.0	C21—C22—C23	121.27 (16)
O1—C7—C8	107.16 (12)	C21—C22—H22	119.4
O1—C7—H7A	110.3	C23—C22—H22	119.4
C8—C7—H7A	110.3	C22—C23—C18	119.23 (15)
O1—C7—H7B	110.3	C22—C23—H23	120.4
C8—C7—H7B	110.3	C18—C23—H23	120.4
C8—N1—N2—C9	−0.32 (16)	N1—N2—C9—N3	0.68 (16)
C7—O1—C1—C2	28.4 (2)	N1—N2—C9—S1	−177.94 (11)
C7—O1—C1—C6	−153.50 (14)	C8—N3—C9—N2	−0.75 (15)
O1—C1—C2—C3	175.06 (16)	C10—N3—C9—N2	177.55 (12)
C6—C1—C2—C3	−3.0 (3)	C8—N3—C9—S1	177.94 (10)
C1—C2—C3—C4	1.2 (3)	C10—N3—C9—S1	−3.76 (19)
C2—C3—C4—C5	1.0 (3)	C16—S1—C9—N2	2.70 (15)
C2—C3—C4—Cl1	−176.55 (15)	C16—S1—C9—N3	−175.77 (12)
C3—C4—C5—C6	−1.3 (3)	C8—N3—C10—C11	−117.80 (16)
Cl1—C4—C5—C6	176.23 (14)	C9—N3—C10—C11	64.27 (19)
C4—C5—C6—C1	−0.5 (3)	C8—N3—C10—C15	61.47 (18)
O1—C1—C6—C5	−175.53 (16)	C9—N3—C10—C15	−116.46 (15)
C2—C1—C6—C5	2.7 (3)	C15—C10—C11—C12	0.3 (2)
C7—O1—C1A—C2A	−40.3 (19)	N3—C10—C11—C12	179.60 (13)
C7—O1—C1A—C6A	154.0 (11)	C10—C11—C12—C13	−1.2 (2)
C6A—C1A—C2A—C3A	0.0	C11—C12—C13—C14	0.8 (2)
O1—C1A—C2A—C3A	−166 (2)	C12—C13—C14—C15	0.5 (2)
C1A—C2A—C3A—C4A	0.0	C11—C10—C15—C14	0.9 (2)
C2A—C3A—C4A—C5A	0.0	N3—C10—C15—C14	−178.32 (13)
C2A—C3A—C4A—Cl1	175 (2)	C13—C14—C15—C10	−1.4 (2)
C3A—C4A—C5A—C6A	0.0	C9—S1—C16—C17	162.90 (11)
Cl1—C4A—C5A—C6A	−173 (3)	C18—N4—C17—O2	−5.4 (2)
C4A—C5A—C6A—C1A	0.0	C18—N4—C17—C16	173.55 (13)
C2A—C1A—C6A—C5A	0.0	S1—C16—C17—O2	10.32 (18)
O1—C1A—C6A—C5A	166 (2)	S1—C16—C17—N4	−168.65 (10)
C1—O1—C7—C8	169.54 (13)	C17—N4—C18—C23	22.5 (2)
C1A—O1—C7—C8	−175.2 (13)	C17—N4—C18—C19	−157.94 (14)
N2—N1—C8—N3	−0.15 (16)	C23—C18—C19—C20	0.2 (2)
N2—N1—C8—C7	178.55 (13)	N4—C18—C19—C20	−179.40 (14)
C9—N3—C8—N1	0.54 (16)	C18—C19—C20—C21	−0.1 (2)
C10—N3—C8—N1	−177.78 (13)	C19—C20—C21—C22	0.3 (3)
C9—N3—C8—C7	−178.17 (13)	C20—C21—C22—C23	−0.6 (3)
C10—N3—C8—C7	3.5 (2)	C21—C22—C23—C18	0.7 (2)
O1—C7—C8—N1	103.81 (16)	C19—C18—C23—C22	−0.5 (2)

O1—C7—C8—N3	−77.67 (17)	N4—C18—C23—C22	179.06 (14)

Hydrogen-bond geometry (Å, º)

Cg3 and Cg4 are the centroids of the C10–C15 and C18–C23 phenyl rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4···N1[i]	0.91	2.02	2.9230 (17)	174
C7—H7*B*···O2[ii]	0.99	2.49	3.3518 (18)	146
C3—H3···*Cg*3[iii]	0.95	2.92	3.867 (2)	174
C15—H15···*Cg*4[iv]	0.95	2.86	3.6871 (16)	146
C16—H16*A*···*Cg*4[v]	0.99	2.80	3.6488 (18)	144

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