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N′-Benzylidene-2-({5-[(4-chlorophenoxy)methyl]-4-phenyl-4*H*-1,2,4-triazol-3-yl}sulfanyl)acetohydrazide hemihydrate

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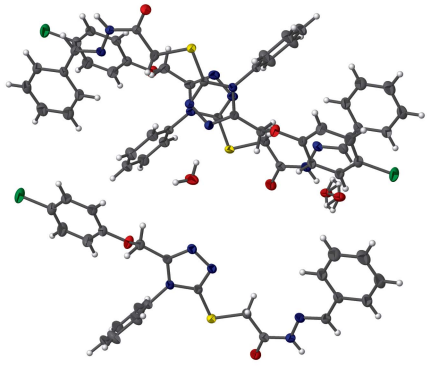
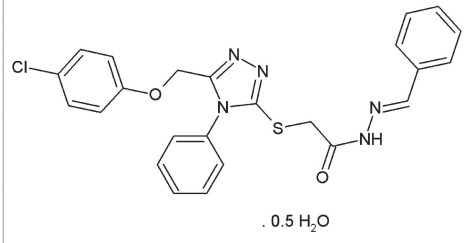
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{24}H_{20}ClN_5O_2S\cdot0.5H_2O$, has three independent molecules in the asymmetric unit and two water molecules of crystallization, one of which is equally disordered over two sites. The three unique organic molecules differ in the conformations of the substituents on the pyrazole ring. In the crystal, extensive O—H···O, O—H···N, N—H···O and C—H···O hydrogen bonding generates a three-dimensional network and C—H···π interactions are also observed.

3D view



Chemical scheme



Structure description

1,2,4-Triazole derivatives are known to exhibit antibacterial, antifungal, antitubercular and anticancer properties (Godhani *et al.*, 2015). They also display anti-inflammatory, anticonvulsant, analagesic and antiviral effects (Godhani *et al.*, 2015). We report here the synthesis and crystal structure of the title 1,2,4-triazole compound.

The asymmetric unit consists of three independent molecules (Figs. 1, 2 and 3) which differ in the conformations of the substituents on the pyrazole ring (Table 1). In addition, there are two water molecules of crystallization, one of which is equally disordered over two sites. The packing involves a extensive three-dimensional network of O—H···O, O—H···N, N—H···O and C—H···O hydrogen bonds (Table 2). C—H···π interactions are also observed.

Table 1
A comparison of the dihedral angles (°) between the ring planes in the three independent molecules in the asymmetric unit of the title compound.

*Cg*1, *Cg*5 and *Cg*9 are the centroids of the 1,2,4-triazole (N1–N3/C8/C9, N6–N8/C32/C33 and N11–N13/C56/C63) rings, *Cg*2, *Cg*6 and *Cg*10 are the centroids of the chlorophenyl (C1–C6, C25–C30 and C49–C54) rings and *Cg*4, *Cg*8 and *Cg*12 are the centroids of the phenyl (C19–C24, C43–C48 and C67–C72) rings.

	*Cg*1^*Cg*2	*Cg*1^*Cg*3	*Cg*1^*Cg*4	*Cg*2^*Cg*3	*Cg*3^*Cg*4
Molecule 1	29.81 (9)	71.56 (9)	22.16 (9)	69.04 (9)	71.67 (9)
	*Cg*5^*Cg*6	*Cg*5^*Cg*7	*Cg*5^*Cg*8	*Cg*6^*Cg*7	*Cg*7^*Cg*8
Molecule 2	30.04 (9)	77.93 (9)	20.61 (9)	78.40 (9)	85.12 (10)
	*Cg*9^*Cg*10	*Cg*9^*Cg*11	*Cg*9^*Cg*12	*Cg*10^*Cg*11	*Cg*11^*Cg*12
Molecule 3	36.44 (9)	67.00 (9)	20.53 (9)	63.12 (9)	69.55 (9)

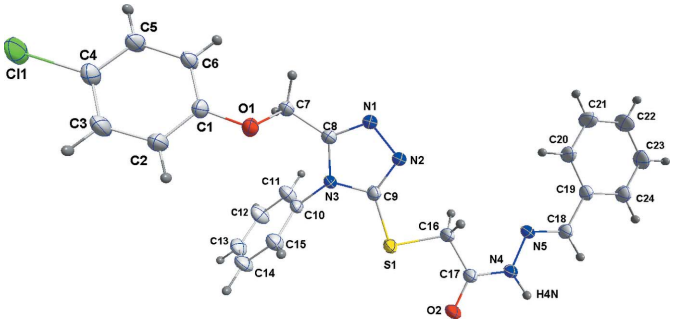


Figure 1
Molecule 1 with the atom-labeling scheme and 50% probability ellipsoids.

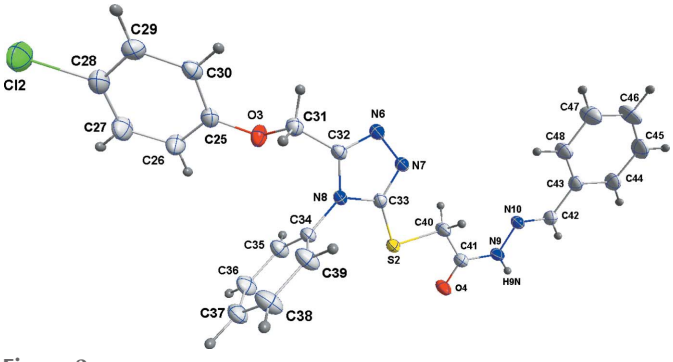


Figure 2
Molecule 2 with the atom-labeling scheme and 50% probability ellipsoids.

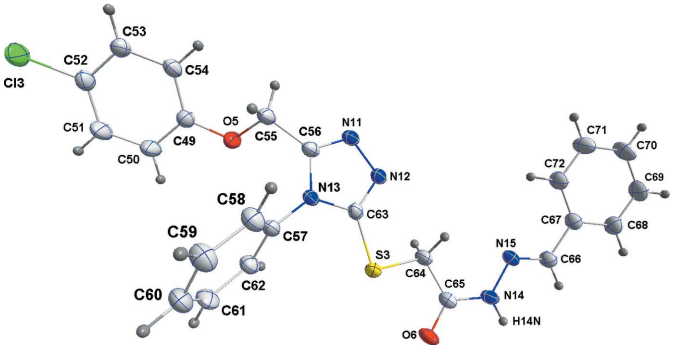


Figure 3
Molecule 3 with the atom-labeling scheme and 50% probability ellipsoids.

Table 2
Hydrogen-bond geometry (Å, °).

*Cg*1 and *Cg*9 are the centroids of the 1,2,4-triazole rings N1–N3/C8/C9 and N11–N13/C56/C63, *Cg*2 and *Cg*10 are the centroids of the chlorophenyl rings C1–C6 and C49–C54, and *Cg*4 and *Cg*12 are the centroids of the phenyl rings C19–C24 and C67–C72.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4*N*···O7^{i}	0.91	1.86	2.7527 (19)	166
C6—H6···O2^{ii}	0.95	2.36	3.2815 (19)	163
C7—H7*A*···O2^{ii}	0.99	2.35	3.304 (2)	162
C30—H30···O4^{i}	0.95	2.48	3.395 (2)	161
C31—H31*B*···O4^{i}	0.99	2.44	3.419 (2)	170
C39—H39···N6^{iii}	0.95	2.51	3.386 (2)	154
N14—H14*N*···O8	0.91	1.98	2.802 (3)	149
C54—H54···O6^{i}	0.95	2.41	3.329 (2)	163
C55—H55*B*···O6^{i}	0.99	2.35	3.254 (2)	151
O7—H7*D*···O4^{i}	0.87	2.14	2.9668 (19)	160
O7—H7*C*···N1	0.87	1.96	2.8239 (19)	176
O8—H8*A*···N11^{ii}	0.87	2.05	2.897 (3)	164
O8—H8*B*···N11^{iv}	0.87	2.16	2.853 (3)	136
C15—H15···*Cg*8^{i}	0.95	2.74	3.670 (2)	168
C35—H35···*Cg*4^{ii}	0.95	2.77	3.709 (2)	169
C62—H62···*Cg*12^{iv}	0.95	2.81	3.714 (2)	159

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

Table 3
Experimental details.

Crystal data	
Chemical formula	$2C_{24}H_{20}ClN_5O_2S\cdot H_2O$
M_r	973.93
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	150
a, *b*, *c* (Å)	10.7330 (4), 16.0616 (6), 20.9885 (8)
α, β, γ (°)	96.662 (2), 102.673 (1), 98.067 (1)
V (Å^3)	3454.5 (2)
Z	3
Radiation type	Cu *K*α
μ (mm^{-1})	2.61
Crystal size (mm)	0.19 × 0.14 × 0.10
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.70, 0.78
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	26548, 12824, 10286
R_{int}	0.029
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.618
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.040, 0.115, 1.02
No. of reflections	12824
No. of parameters	910
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.36, −0.36

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

Synthesis and crystallization

An equimolar mixture of 5-[(4-chlorophenoxy)methyl-4-phenyl-4*H*-1,2,4-triazol-3-ylthio], acetohydrazide and benzaldehyde (10 mmol) in ethanol (20 ml) was heated under reflux for 2 h and then allowed to cool. The solid that separated was

collected and recrystallized from water/ethanol (1:1 *v*/*v*) solution. Yield: 86%; m.p.: 445-446 K. IR (KBr) ν = 3200 (NH), 1670 (C═O) cm.$^{-1}$ ^{1}NMR ($CDCl_3$): δ 11.0 (*s*, 1H, NH), 7.00–7.80 (15*H*, Ar H and N═CH), 4.95 (*s*, 2H, OCH_2), 4.00 (*s*, 2H, SCH_2) p.p.m.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The O8 water molecule is equally disordered over two sites.

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x160627 [doi:10.1107/S2414314616006271]

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_N_′-Benzylidene-2-({5-[(4-chlorophenoxy)methyl]-4-phenyl-4*H*-1,2,4-triazol-3-yl}sulfanyl)acetohydrazide hemihydrate

Crystal data

$2C_{24}H_{20}ClN_5O_2S·H_2O$
M_r = 973.93
Triclinic, $P\overline{1}$
a = 10.7330 (4) Å
b = 16.0616 (6) Å
c = 20.9885 (8) Å
α = 96.662 (2)°
β = 102.673 (1)°
γ = 98.067 (1)°
V = 3454.5 (2) Å^3
Z = 3
$F(000)$ = 1518
D_x = 1.404 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9989 reflections
θ = 4.3–72.3°
μ = 2.61 mm^{-1}
T = 150 K
Block, colourless
0.19 × 0.14 × 0.10 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} = 0.70, T_{max} = 0.78
26548 measured reflections
12824 independent reflections
10286 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 72.3°, θ_{min} = 3.3°
h = −11→13
k = −18→19
l = −25→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.115
S = 1.02
12824 reflections
910 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
$w = 1/[\sigma^2(F_o^2) + (0.0615P)^2 + 0.7789P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 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.

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 $F^2 > 2\text{sigma}(F^2)$ 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 - 0.98 Å) while those attached to nitrogen and oxygen were placed in locations derived from a difference map and their parameters adjusted to give N—H = 0.91 and O—H = 0.87 Å. All were included as riding contributions with isotropic displacement parameters 1.2 - 1.5 times those of the attached atoms.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cl1	0.12794 (4)	0.02365 (3)	0.07115 (2)	0.03665 (12)	
S1	1.12202 (4)	0.39667 (3)	0.18914 (2)	0.02712 (11)	
O1	0.61710 (11)	0.26313 (7)	0.17608 (6)	0.0274 (3)	
O2	1.39656 (11)	0.42943 (7)	0.22596 (6)	0.0295 (3)	
N1	0.81198 (13)	0.45379 (9)	0.23687 (7)	0.0231 (3)	
N2	0.94582 (13)	0.46910 (8)	0.24447 (7)	0.0224 (3)	
N3	0.85927 (13)	0.36096 (8)	0.16435 (7)	0.0208 (3)	
N4	1.43515 (13)	0.56242 (8)	0.28161 (7)	0.0222 (3)	
H4N	1.5221	0.5628	0.2907	0.027*	
N5	1.38571 (13)	0.63073 (8)	0.30537 (6)	0.0211 (3)	
C1	0.49880 (16)	0.21077 (10)	0.15014 (8)	0.0234 (3)	
C2	0.50334 (17)	0.12681 (11)	0.12928 (10)	0.0336 (4)	
H2	0.5846	0.1088	0.1316	0.040*	
C3	0.38907 (18)	0.06848 (11)	0.10493 (10)	0.0363 (4)	
H3	0.3916	0.0106	0.0904	0.044*	
C4	0.27209 (17)	0.09580 (11)	0.10214 (9)	0.0273 (4)	
C5	0.26675 (16)	0.17952 (11)	0.12284 (8)	0.0260 (4)	
H5	0.1853	0.1972	0.1208	0.031*	
C6	0.38112 (16)	0.23825 (10)	0.14684 (8)	0.0235 (3)	
H6	0.3784	0.2963	0.1607	0.028*	
C7	0.62368 (15)	0.35041 (10)	0.16693 (8)	0.0239 (3)	
H7A	0.5718	0.3792	0.1934	0.029*	
H7B	0.5899	0.3548	0.1198	0.029*	
C8	0.76254 (15)	0.38988 (10)	0.18931 (8)	0.0215 (3)	
C9	0.97106 (15)	0.41238 (10)	0.20090 (8)	0.0212 (3)	
C10	0.84291 (15)	0.30157 (10)	0.10504 (8)	0.0219 (3)	
C11	0.7900 (2)	0.32576 (11)	0.04546 (9)	0.0336 (4)	
H11	0.7652	0.3802	0.0440	0.040*	
C12	0.7733 (2)	0.26933 (13)	−0.01246 (9)	0.0396 (5)	
H12	0.7362	0.2849	−0.0538	0.048*	
C13	0.81049 (19)	0.19077 (12)	−0.00990 (9)	0.0343 (4)	
H13	0.7990	0.1523	−0.0495	0.041*	

C14	0.86450 (19)	0.16782 (11)	0.05028 (10)	0.0352 (4)
H14	0.8905	0.1138	0.0517	0.042*
C15	0.88101 (18)	0.22337 (11)	0.10867 (9)	0.0295 (4)
H15	0.9177	0.2078	0.1501	0.035*
C16	1.21388 (16)	0.48887 (11)	0.24583 (9)	0.0302 (4)
H16A	1.1873	0.5412	0.2305	0.036*
H16B	1.1971	0.4865	0.2902	0.036*
C17	1.35506 (15)	0.49070 (10)	0.24946 (8)	0.0211 (3)
C18	1.46994 (16)	0.69472 (10)	0.33807 (8)	0.0230 (3)
H18	1.5596	0.6921	0.3444	0.028*
C19	1.42993 (16)	0.77148 (10)	0.36568 (8)	0.0229 (3)
C20	1.30025 (17)	0.77665 (11)	0.36287 (9)	0.0312 (4)
H20	1.2349	0.7286	0.3435	0.037*
C21	1.2662 (2)	0.85122 (13)	0.38814 (11)	0.0409 (5)
H21	1.1776	0.8541	0.3860	0.049*
C22	1.3608 (2)	0.92209 (12)	0.41674 (10)	0.0401 (5)
H22	1.3368	0.9733	0.4338	0.048*
C23	1.48956 (19)	0.91764 (11)	0.42014 (9)	0.0337 (4)
H23	1.5545	0.9658	0.4398	0.040*
C24	1.52427 (17)	0.84294 (11)	0.39491 (8)	0.0279 (4)
H24	1.6131	0.8403	0.3975	0.033*
Cl2	1.19206 (5)	0.96964 (3)	0.58780 (3)	0.04395 (13)
S2	0.18741 (4)	0.60384 (3)	0.46784 (2)	0.02689 (11)
O3	0.69930 (11)	0.73152 (7)	0.49432 (7)	0.0311 (3)
O4	−0.08883 (12)	0.55580 (8)	0.43783 (7)	0.0344 (3)
N6	0.50482 (13)	0.54226 (8)	0.43110 (7)	0.0233 (3)
N7	0.36993 (13)	0.52876 (8)	0.41977 (7)	0.0229 (3)
N8	0.45090 (13)	0.63731 (8)	0.50012 (7)	0.0214 (3)
N9	−0.11306 (14)	0.42286 (9)	0.38391 (7)	0.0268 (3)
H9N	−0.1999	0.4150	0.3808	0.032*
N10	−0.05591 (14)	0.36018 (9)	0.35767 (7)	0.0241 (3)
C25	0.81876 (16)	0.78290 (11)	0.51779 (8)	0.0258 (4)
C26	0.81619 (18)	0.86787 (12)	0.53677 (11)	0.0374 (5)
H26	0.7357	0.8867	0.5353	0.045*
C27	0.93163 (19)	0.92568 (12)	0.55800 (11)	0.0406 (5)
H27	0.9305	0.9842	0.5711	0.049*
C28	1.04733 (18)	0.89747 (11)	0.55992 (9)	0.0309 (4)
C29	1.05050 (17)	0.81287 (11)	0.54099 (9)	0.0297 (4)
H29	1.1311	0.7943	0.5423	0.036*
C30	0.93536 (17)	0.75464 (11)	0.51990 (9)	0.0269 (4)
H30	0.9368	0.6961	0.5071	0.032*
C31	0.68888 (16)	0.64487 (10)	0.50496 (9)	0.0251 (3)
H31A	0.7167	0.6416	0.5527	0.030*
H31B	0.7439	0.6148	0.4813	0.030*
C32	0.55014 (16)	0.60631 (10)	0.47883 (8)	0.0216 (3)
C33	0.34104 (16)	0.58642 (10)	0.46116 (8)	0.0218 (3)
C34	0.46277 (16)	0.69535 (10)	0.55969 (8)	0.0225 (3)
C35	0.44295 (18)	0.77783 (11)	0.55637 (9)	0.0304 (4)

H35	0.4186	0.7969	0.5149	0.037*
C36	0.45946 (19)	0.83255 (11)	0.61530 (9)	0.0339 (4)
H36	0.4458	0.8896	0.6141	0.041*
C37	0.49558 (18)	0.80473 (11)	0.67547 (9)	0.0320 (4)
H37	0.5085	0.8429	0.7154	0.038*
C38	0.5128 (2)	0.72143 (12)	0.67754 (9)	0.0390 (5)
H38	0.5364	0.7021	0.7189	0.047*
C39	0.4957 (2)	0.66584 (11)	0.61924 (9)	0.0343 (4)
H39	0.5064	0.6083	0.6204	0.041*
C40	0.10066 (16)	0.50658 (11)	0.41584 (9)	0.0289 (4)
H40A	0.1129	0.5070	0.3705	0.035*
H40B	0.1351	0.4574	0.4330	0.035*
C41	−0.04021 (16)	0.49811 (10)	0.41444 (8)	0.0244 (3)
C42	−0.13140 (17)	0.29249 (10)	0.32632 (8)	0.0267 (4)
H42	−0.2223	0.2877	0.3218	0.032*
C43	−0.07855 (17)	0.22218 (11)	0.29736 (8)	0.0267 (4)
C44	−0.16151 (19)	0.14566 (11)	0.26911 (9)	0.0335 (4)
H44	−0.2513	0.1404	0.2678	0.040*
C45	−0.1132 (2)	0.07711 (12)	0.24294 (10)	0.0416 (5)
H45	−0.1697	0.0248	0.2245	0.050*
C46	0.0165 (2)	0.08484 (13)	0.24367 (11)	0.0470 (5)
H46	0.0491	0.0380	0.2252	0.056*
C47	0.1001 (2)	0.16111 (13)	0.27134 (11)	0.0436 (5)
H47	0.1895	0.1663	0.2716	0.052*
C48	0.05301 (18)	0.22924 (12)	0.29835 (9)	0.0330 (4)
H48	0.1103	0.2810	0.3176	0.040*
Cl3	1.55953 (5)	0.98118 (3)	0.25967 (3)	0.03985 (12)
S3	0.56870 (4)	0.60125 (3)	0.15171 (2)	0.02948 (11)
O5	1.06779 (12)	0.74449 (7)	0.15696 (6)	0.0301 (3)
O6	0.29150 (13)	0.56880 (8)	0.11686 (7)	0.0385 (3)
N11	0.87392 (15)	0.55264 (9)	0.09435 (7)	0.0290 (3)
N12	0.74092 (14)	0.53513 (9)	0.08974 (7)	0.0275 (3)
N13	0.82988 (14)	0.64258 (8)	0.17018 (7)	0.0242 (3)
N14	0.25687 (14)	0.43728 (9)	0.05974 (7)	0.0287 (3)
H14N	0.1704	0.4324	0.0573	0.034*
N15	0.30451 (14)	0.37172 (9)	0.03053 (7)	0.0259 (3)
C49	1.18680 (17)	0.79586 (11)	0.18190 (8)	0.0257 (4)
C50	1.18353 (18)	0.88119 (11)	0.19813 (10)	0.0350 (4)
H50	1.1026	0.9004	0.1928	0.042*
C51	1.29814 (19)	0.93896 (12)	0.22214 (10)	0.0366 (4)
H51	1.2964	0.9977	0.2337	0.044*
C52	1.41518 (18)	0.90970 (11)	0.22904 (9)	0.0296 (4)
C53	1.41869 (17)	0.82472 (11)	0.21257 (8)	0.0273 (4)
H53	1.4997	0.8057	0.2173	0.033*
C54	1.30403 (17)	0.76661 (11)	0.18907 (8)	0.0258 (4)
H54	1.3059	0.7078	0.1781	0.031*
C55	1.06298 (17)	0.65642 (10)	0.16225 (9)	0.0289 (4)
H55A	1.1013	0.6493	0.2083	0.035*

H55B	1.1122	0.6301	0.1330	0.035*	
C56	0.92447 (17)	0.61592 (10)	0.14220 (9)	0.0256 (4)	
C57	0.84799 (16)	0.70182 (10)	0.22982 (8)	0.0243 (3)	
C58	0.91552 (18)	0.68166 (11)	0.28860 (9)	0.0323 (4)	
H58	0.9507	0.6306	0.2890	0.039*	
C59	0.9313 (2)	0.73692 (12)	0.34699 (9)	0.0369 (4)	
H59	0.9777	0.7239	0.3876	0.044*	
C60	0.87920 (19)	0.81097 (12)	0.34580 (10)	0.0361 (4)	
H60	0.8890	0.8484	0.3858	0.043*	
C61	0.81292 (19)	0.83065 (12)	0.28665 (10)	0.0356 (4)	
H61	0.7782	0.8819	0.2862	0.043*	
C62	0.79669 (18)	0.77612 (11)	0.22779 (9)	0.0306 (4)	
H62	0.7514	0.7896	0.1871	0.037*	
C63	0.71809 (17)	0.59024 (10)	0.13520 (8)	0.0244 (3)	
C64	0.47291 (17)	0.52112 (11)	0.08542 (9)	0.0313 (4)	
H64A	0.4811	0.5379	0.0424	0.038*	
H64B	0.5042	0.4663	0.0890	0.038*	
C65	0.33429 (17)	0.51129 (11)	0.08923 (8)	0.0257 (4)	
C66	0.21972 (17)	0.30648 (11)	0.00079 (8)	0.0282 (4)	
H66	0.1309	0.3067	−0.0001	0.034*	
C67	0.25762 (17)	0.23198 (11)	−0.03162 (8)	0.0268 (4)	
C68	0.16250 (19)	0.16047 (12)	−0.05987 (9)	0.0327 (4)	
H68	0.0748	0.1618	−0.0588	0.039*	
C69	0.1956 (2)	0.08767 (12)	−0.08947 (10)	0.0379 (5)	
H69	0.1306	0.0392	−0.1082	0.045*	
C70	0.3225 (2)	0.08541 (12)	−0.09173 (10)	0.0414 (5)	
H70	0.3450	0.0355	−0.1120	0.050*	
C71	0.4177 (2)	0.15634 (13)	−0.06434 (11)	0.0413 (5)	
H71	0.5050	0.1549	−0.0662	0.050*	
C72	0.38555 (18)	0.22881 (12)	−0.03444 (9)	0.0333 (4)	
H72	0.4511	0.2769	−0.0156	0.040*	
O7	0.69091 (13)	0.54516 (11)	0.32193 (7)	0.0521 (4)	
H7D	0.7463	0.5584	0.3601	0.078*	
H7C	0.7313	0.5176	0.2971	0.078*	
O8	−0.0028 (3)	0.45181 (17)	0.01102 (13)	0.0399 (6)	0.5
H8A	−0.0358	0.4901	0.0315	0.060*	0.5
H8B	0.0176	0.4753	−0.0215	0.060*	0.5

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0285 (2)	0.0246 (2)	0.0484 (3)	−0.00373 (16)	0.00048 (19)	−0.00218 (19)
S1	0.0215 (2)	0.0229 (2)	0.0349 (2)	−0.00075 (15)	0.01176 (17)	−0.00797 (17)
O1	0.0212 (6)	0.0212 (6)	0.0368 (7)	0.0024 (4)	0.0016 (5)	0.0038 (5)
O2	0.0255 (6)	0.0239 (6)	0.0384 (7)	0.0071 (5)	0.0099 (5)	−0.0062 (5)
N1	0.0202 (7)	0.0225 (7)	0.0258 (7)	0.0043 (5)	0.0059 (6)	−0.0012 (6)
N2	0.0199 (7)	0.0210 (7)	0.0257 (7)	0.0036 (5)	0.0068 (6)	−0.0017 (6)
N3	0.0210 (7)	0.0179 (6)	0.0225 (7)	0.0023 (5)	0.0061 (5)	−0.0020 (5)

N4	0.0192 (7)	0.0215 (7)	0.0253 (7)	0.0037 (5)	0.0066 (6)	−0.0018 (6)
N5	0.0244 (7)	0.0186 (6)	0.0209 (6)	0.0054 (5)	0.0065 (5)	0.0012 (5)
C1	0.0209 (8)	0.0233 (8)	0.0237 (8)	0.0011 (6)	0.0030 (6)	0.0012 (7)
C2	0.0249 (9)	0.0244 (9)	0.0492 (11)	0.0059 (7)	0.0070 (8)	−0.0019 (8)
C3	0.0334 (10)	0.0197 (8)	0.0522 (12)	0.0042 (7)	0.0084 (9)	−0.0046 (8)
C4	0.0270 (9)	0.0226 (8)	0.0288 (9)	−0.0004 (6)	0.0036 (7)	0.0011 (7)
C5	0.0210 (8)	0.0261 (8)	0.0285 (9)	0.0052 (6)	0.0020 (7)	0.0008 (7)
C6	0.0245 (8)	0.0198 (8)	0.0241 (8)	0.0041 (6)	0.0033 (7)	−0.0014 (7)
C7	0.0214 (8)	0.0195 (8)	0.0300 (9)	0.0051 (6)	0.0048 (7)	0.0012 (7)
C8	0.0222 (8)	0.0192 (7)	0.0230 (8)	0.0050 (6)	0.0058 (6)	0.0008 (6)
C9	0.0222 (8)	0.0172 (7)	0.0238 (8)	0.0012 (6)	0.0067 (6)	0.0021 (6)
C10	0.0223 (8)	0.0198 (8)	0.0221 (8)	0.0007 (6)	0.0073 (6)	−0.0030 (6)
C11	0.0498 (12)	0.0241 (9)	0.0275 (9)	0.0115 (8)	0.0089 (8)	0.0011 (7)
C12	0.0594 (13)	0.0358 (10)	0.0231 (9)	0.0134 (9)	0.0075 (9)	0.0000 (8)
C13	0.0432 (11)	0.0294 (9)	0.0283 (9)	0.0058 (8)	0.0104 (8)	−0.0069 (8)
C14	0.0449 (11)	0.0233 (9)	0.0374 (10)	0.0121 (8)	0.0104 (9)	−0.0042 (8)
C15	0.0369 (10)	0.0232 (8)	0.0275 (9)	0.0082 (7)	0.0056 (8)	0.0008 (7)
C16	0.0203 (8)	0.0251 (8)	0.0413 (10)	0.0034 (6)	0.0068 (7)	−0.0093 (8)
C17	0.0220 (8)	0.0198 (8)	0.0217 (8)	0.0046 (6)	0.0061 (6)	0.0015 (6)
C18	0.0209 (8)	0.0225 (8)	0.0246 (8)	0.0017 (6)	0.0053 (6)	0.0025 (7)
C19	0.0268 (8)	0.0200 (8)	0.0203 (8)	0.0033 (6)	0.0035 (7)	0.0013 (6)
C20	0.0256 (9)	0.0272 (9)	0.0361 (10)	0.0026 (7)	0.0031 (7)	−0.0041 (8)
C21	0.0325 (10)	0.0352 (10)	0.0506 (12)	0.0106 (8)	0.0042 (9)	−0.0068 (9)
C22	0.0471 (12)	0.0247 (9)	0.0449 (11)	0.0113 (8)	0.0055 (9)	−0.0049 (9)
C23	0.0398 (11)	0.0210 (8)	0.0337 (10)	−0.0014 (7)	0.0025 (8)	−0.0023 (8)
C24	0.0273 (9)	0.0244 (8)	0.0289 (9)	0.0004 (7)	0.0037 (7)	0.0022 (7)
Cl2	0.0309 (2)	0.0311 (2)	0.0600 (3)	−0.00541 (18)	−0.0001 (2)	0.0009 (2)
S2	0.0252 (2)	0.0215 (2)	0.0330 (2)	0.00191 (15)	0.01075 (17)	−0.00469 (17)
O3	0.0234 (6)	0.0204 (6)	0.0458 (8)	0.0027 (5)	0.0000 (5)	0.0074 (5)
O4	0.0289 (7)	0.0303 (7)	0.0423 (7)	0.0089 (5)	0.0099 (6)	−0.0088 (6)
N6	0.0246 (7)	0.0213 (7)	0.0233 (7)	0.0045 (5)	0.0051 (6)	0.0010 (6)
N7	0.0254 (7)	0.0207 (7)	0.0224 (7)	0.0039 (5)	0.0066 (6)	0.0010 (6)
N8	0.0228 (7)	0.0185 (6)	0.0215 (7)	0.0025 (5)	0.0051 (5)	−0.0014 (5)
N9	0.0238 (7)	0.0246 (7)	0.0318 (8)	0.0044 (5)	0.0100 (6)	−0.0026 (6)
N10	0.0287 (7)	0.0208 (7)	0.0237 (7)	0.0059 (5)	0.0079 (6)	0.0015 (6)
C25	0.0247 (8)	0.0241 (8)	0.0259 (8)	0.0026 (6)	0.0023 (7)	0.0024 (7)
C26	0.0262 (9)	0.0261 (9)	0.0556 (12)	0.0077 (7)	0.0040 (9)	−0.0039 (9)
C27	0.0349 (11)	0.0227 (9)	0.0573 (13)	0.0042 (7)	0.0027 (9)	−0.0048 (9)
C28	0.0289 (9)	0.0268 (9)	0.0323 (9)	−0.0004 (7)	0.0013 (7)	0.0028 (8)
C29	0.0251 (9)	0.0309 (9)	0.0325 (9)	0.0065 (7)	0.0060 (7)	0.0027 (8)
C30	0.0290 (9)	0.0210 (8)	0.0302 (9)	0.0055 (7)	0.0065 (7)	0.0013 (7)
C31	0.0233 (8)	0.0213 (8)	0.0293 (9)	0.0051 (6)	0.0038 (7)	0.0022 (7)
C32	0.0259 (8)	0.0173 (7)	0.0224 (8)	0.0053 (6)	0.0069 (7)	0.0018 (6)
C33	0.0254 (8)	0.0183 (7)	0.0212 (8)	0.0023 (6)	0.0059 (7)	0.0019 (6)
C34	0.0238 (8)	0.0203 (8)	0.0228 (8)	0.0035 (6)	0.0073 (6)	−0.0025 (7)
C35	0.0421 (11)	0.0232 (8)	0.0261 (9)	0.0081 (7)	0.0074 (8)	0.0026 (7)
C36	0.0462 (11)	0.0198 (8)	0.0364 (10)	0.0100 (7)	0.0115 (9)	−0.0015 (8)
C37	0.0375 (10)	0.0287 (9)	0.0270 (9)	0.0060 (7)	0.0077 (8)	−0.0067 (7)

C38	0.0609 (14)	0.0339 (10)	0.0232 (9)	0.0173 (9)	0.0086 (9)	0.0000 (8)
C39	0.0527 (12)	0.0245 (9)	0.0266 (9)	0.0145 (8)	0.0082 (8)	0.0006 (7)
C40	0.0236 (8)	0.0295 (9)	0.0301 (9)	0.0050 (7)	0.0049 (7)	−0.0071 (7)
C41	0.0278 (9)	0.0236 (8)	0.0222 (8)	0.0072 (6)	0.0055 (7)	0.0021 (7)
C42	0.0263 (9)	0.0236 (8)	0.0295 (9)	0.0020 (6)	0.0078 (7)	0.0019 (7)
C43	0.0324 (9)	0.0229 (8)	0.0232 (8)	0.0027 (7)	0.0056 (7)	0.0018 (7)
C44	0.0367 (10)	0.0266 (9)	0.0326 (10)	−0.0008 (7)	0.0061 (8)	−0.0014 (8)
C45	0.0542 (13)	0.0232 (9)	0.0412 (11)	0.0001 (8)	0.0082 (10)	−0.0058 (8)
C46	0.0566 (14)	0.0323 (11)	0.0499 (13)	0.0178 (9)	0.0095 (11)	−0.0087 (10)
C47	0.0374 (11)	0.0392 (11)	0.0510 (13)	0.0126 (9)	0.0060 (10)	−0.0044 (10)
C48	0.0326 (10)	0.0278 (9)	0.0347 (10)	0.0049 (7)	0.0044 (8)	−0.0036 (8)
Cl3	0.0333 (2)	0.0263 (2)	0.0529 (3)	0.00035 (17)	0.0026 (2)	−0.0022 (2)
S3	0.0289 (2)	0.0275 (2)	0.0315 (2)	−0.00109 (16)	0.01585 (18)	−0.00690 (18)
O5	0.0264 (6)	0.0218 (6)	0.0417 (7)	0.0053 (5)	0.0062 (5)	0.0055 (5)
O6	0.0343 (7)	0.0346 (7)	0.0445 (8)	0.0133 (6)	0.0096 (6)	−0.0115 (6)
N11	0.0312 (8)	0.0249 (7)	0.0344 (8)	0.0077 (6)	0.0151 (7)	0.0010 (6)
N12	0.0311 (8)	0.0225 (7)	0.0313 (8)	0.0042 (6)	0.0145 (6)	0.0007 (6)
N13	0.0274 (7)	0.0189 (6)	0.0281 (7)	0.0035 (5)	0.0120 (6)	0.0009 (6)
N14	0.0276 (8)	0.0289 (8)	0.0291 (8)	0.0078 (6)	0.0082 (6)	−0.0041 (6)
N15	0.0320 (8)	0.0230 (7)	0.0227 (7)	0.0080 (6)	0.0065 (6)	−0.0003 (6)
C49	0.0265 (9)	0.0249 (8)	0.0259 (8)	0.0049 (6)	0.0062 (7)	0.0042 (7)
C50	0.0310 (10)	0.0260 (9)	0.0484 (11)	0.0108 (7)	0.0087 (9)	0.0017 (8)
C51	0.0373 (11)	0.0218 (9)	0.0500 (12)	0.0090 (7)	0.0097 (9)	−0.0009 (8)
C52	0.0310 (9)	0.0250 (9)	0.0299 (9)	0.0026 (7)	0.0040 (7)	0.0007 (7)
C53	0.0267 (9)	0.0295 (9)	0.0255 (8)	0.0084 (7)	0.0049 (7)	0.0017 (7)
C54	0.0300 (9)	0.0212 (8)	0.0266 (8)	0.0072 (7)	0.0072 (7)	0.0014 (7)
C55	0.0284 (9)	0.0213 (8)	0.0398 (10)	0.0080 (7)	0.0122 (8)	0.0040 (7)
C56	0.0292 (9)	0.0207 (8)	0.0312 (9)	0.0078 (6)	0.0134 (7)	0.0048 (7)
C57	0.0257 (8)	0.0214 (8)	0.0263 (8)	0.0025 (6)	0.0109 (7)	−0.0012 (7)
C58	0.0383 (10)	0.0254 (9)	0.0336 (10)	0.0093 (7)	0.0084 (8)	0.0023 (8)
C59	0.0447 (11)	0.0339 (10)	0.0299 (10)	0.0080 (8)	0.0057 (8)	−0.0001 (8)
C60	0.0391 (11)	0.0311 (10)	0.0353 (10)	0.0039 (8)	0.0113 (8)	−0.0083 (8)
C61	0.0390 (11)	0.0255 (9)	0.0429 (11)	0.0132 (8)	0.0106 (9)	−0.0037 (8)
C62	0.0348 (10)	0.0246 (9)	0.0334 (10)	0.0083 (7)	0.0099 (8)	0.0006 (8)
C63	0.0300 (9)	0.0186 (8)	0.0262 (8)	0.0013 (6)	0.0122 (7)	0.0029 (7)
C64	0.0312 (10)	0.0288 (9)	0.0335 (9)	0.0071 (7)	0.0104 (8)	−0.0048 (8)
C65	0.0303 (9)	0.0246 (8)	0.0227 (8)	0.0098 (7)	0.0056 (7)	0.0007 (7)
C66	0.0288 (9)	0.0289 (9)	0.0254 (8)	0.0042 (7)	0.0058 (7)	0.0006 (7)
C67	0.0316 (9)	0.0251 (8)	0.0224 (8)	0.0044 (7)	0.0047 (7)	0.0019 (7)
C68	0.0329 (10)	0.0307 (9)	0.0312 (9)	0.0005 (7)	0.0066 (8)	−0.0003 (8)
C69	0.0447 (12)	0.0266 (9)	0.0364 (10)	−0.0004 (8)	0.0052 (9)	−0.0034 (8)
C70	0.0493 (12)	0.0281 (10)	0.0429 (11)	0.0122 (8)	0.0055 (10)	−0.0058 (9)
C71	0.0333 (10)	0.0390 (11)	0.0483 (12)	0.0117 (8)	0.0056 (9)	−0.0048 (9)
C72	0.0310 (10)	0.0297 (9)	0.0341 (10)	0.0030 (7)	0.0030 (8)	−0.0043 (8)
O7	0.0289 (7)	0.0912 (12)	0.0338 (7)	0.0257 (7)	0.0036 (6)	−0.0114 (8)
O8	0.0342 (15)	0.0482 (17)	0.0395 (15)	0.0091 (12)	0.0171 (12)	−0.0027 (13)

Geometric parameters (Å, º)

Cl1—C4	1.7436 (17)	C35—C36	1.393 (2)
S1—C9	1.7394 (16)	C35—H35	0.9500
S1—C16	1.8020 (17)	C36—C37	1.382 (3)
O1—C1	1.3808 (19)	C36—H36	0.9500
O1—C7	1.4309 (19)	C37—C38	1.380 (3)
O2—C17	1.2315 (19)	C37—H37	0.9500
N1—C8	1.307 (2)	C38—C39	1.389 (2)
N1—N2	1.3931 (18)	C38—H38	0.9500
N2—C9	1.313 (2)	C39—H39	0.9500
N3—C9	1.3716 (19)	C40—C41	1.492 (2)
N3—C8	1.373 (2)	C40—H40A	0.9900
N3—C10	1.4394 (19)	C40—H40B	0.9900
N4—C17	1.345 (2)	C42—C43	1.462 (2)
N4—N5	1.3735 (18)	C42—H42	0.9500
N4—H4N	0.9100	C43—C44	1.395 (2)
N5—C18	1.284 (2)	C43—C48	1.396 (3)
C1—C2	1.380 (2)	C44—C45	1.388 (3)
C1—C6	1.386 (2)	C44—H44	0.9500
C2—C3	1.391 (2)	C45—C46	1.377 (3)
C2—H2	0.9500	C45—H45	0.9500
C3—C4	1.379 (3)	C46—C47	1.393 (3)
C3—H3	0.9500	C46—H46	0.9500
C4—C5	1.377 (2)	C47—C48	1.383 (3)
C5—C6	1.394 (2)	C47—H47	0.9500
C5—H5	0.9500	C48—H48	0.9500
C6—H6	0.9500	Cl3—C52	1.7391 (18)
C7—C8	1.484 (2)	S3—C63	1.7412 (17)
C7—H7A	0.9900	S3—C64	1.7986 (18)
C7—H7B	0.9900	O5—C49	1.377 (2)
C10—C11	1.379 (2)	O5—C55	1.426 (2)
C10—C15	1.380 (2)	O6—C65	1.230 (2)
C11—C12	1.391 (2)	N11—C56	1.306 (2)
C11—H11	0.9500	N11—N12	1.395 (2)
C12—C13	1.379 (3)	N12—C63	1.312 (2)
C12—H12	0.9500	N13—C63	1.368 (2)
C13—C14	1.383 (3)	N13—C56	1.373 (2)
C13—H13	0.9500	N13—C57	1.441 (2)
C14—C15	1.391 (2)	N14—C65	1.346 (2)
C14—H14	0.9500	N14—N15	1.3731 (19)
C15—H15	0.9500	N14—H14N	0.9100
C16—C17	1.496 (2)	N15—C66	1.283 (2)
C16—H16A	0.9900	C49—C50	1.381 (2)
C16—H16B	0.9900	C49—C54	1.388 (2)
C18—C19	1.460 (2)	C50—C51	1.388 (3)
C18—H18	0.9500	C50—H50	0.9500
C19—C20	1.395 (2)	C51—C52	1.386 (3)

C19—C24	1.399 (2)	C51—H51	0.9500
C20—C21	1.382 (3)	C52—C53	1.376 (2)
C20—H20	0.9500	C53—C54	1.391 (2)
C21—C22	1.391 (3)	C53—H53	0.9500
C21—H21	0.9500	C54—H54	0.9500
C22—C23	1.381 (3)	C55—C56	1.484 (2)
C22—H22	0.9500	C55—H55A	0.9900
C23—C24	1.387 (2)	C55—H55B	0.9900
C23—H23	0.9500	C57—C62	1.384 (2)
C24—H24	0.9500	C57—C58	1.385 (2)
Cl2—C28	1.7428 (18)	C58—C59	1.390 (2)
S2—C33	1.7431 (17)	C58—H58	0.9500
S2—C40	1.8024 (17)	C59—C60	1.384 (3)
O3—C25	1.378 (2)	C59—H59	0.9500
O3—C31	1.4279 (19)	C60—C61	1.384 (3)
O4—C41	1.231 (2)	C60—H60	0.9500
N6—C32	1.306 (2)	C61—C62	1.391 (2)
N6—N7	1.3958 (19)	C61—H61	0.9500
N7—C33	1.312 (2)	C62—H62	0.9500
N8—C33	1.371 (2)	C64—C65	1.495 (2)
N8—C32	1.374 (2)	C64—H64A	0.9900
N8—C34	1.4404 (19)	C64—H64B	0.9900
N9—C41	1.348 (2)	C66—C67	1.459 (2)
N9—N10	1.3734 (19)	C66—H66	0.9500
N9—H9N	0.9099	C67—C72	1.395 (3)
N10—C42	1.274 (2)	C67—C68	1.400 (2)
C25—C26	1.382 (2)	C68—C69	1.387 (3)
C25—C30	1.384 (2)	C68—H68	0.9500
C26—C27	1.391 (3)	C69—C70	1.380 (3)
C26—H26	0.9500	C69—H69	0.9500
C27—C28	1.374 (3)	C70—C71	1.391 (3)
C27—H27	0.9500	C70—H70	0.9500
C28—C29	1.378 (2)	C71—C72	1.381 (3)
C29—C30	1.392 (2)	C71—H71	0.9500
C29—H29	0.9500	C72—H72	0.9500
C30—H30	0.9500	O7—H7D	0.8699
C31—C32	1.485 (2)	O7—H7C	0.8699
C31—H31A	0.9900	O8—O8^{i}	1.663 (6)
C31—H31B	0.9900	O8—H8A	0.8700
C34—C35	1.378 (2)	O8—H8B	0.8700
C34—C39	1.379 (2)		

C9—S1—C16	96.16 (8)	C36—C35—H35	120.8
C1—O1—C7	116.49 (12)	C37—C36—C35	120.68 (17)
C8—N1—N2	108.17 (13)	C37—C36—H36	119.7
C9—N2—N1	106.36 (12)	C35—C36—H36	119.7
C9—N3—C8	104.54 (13)	C38—C37—C36	119.94 (16)
C9—N3—C10	127.84 (13)	C38—C37—H37	120.0

C8—N3—C10	126.61 (13)	C36—C37—H37	120.0
C17—N4—N5	120.22 (13)	C37—C38—C39	120.11 (18)
C17—N4—H4N	118.6	C37—C38—H38	119.9
N5—N4—H4N	120.9	C39—C38—H38	119.9
C18—N5—N4	115.60 (14)	C34—C39—C38	119.09 (17)
C2—C1—O1	115.90 (15)	C34—C39—H39	120.5
C2—C1—C6	120.75 (15)	C38—C39—H39	120.5
O1—C1—C6	123.30 (15)	C41—C40—S2	109.83 (11)
C1—C2—C3	120.09 (17)	C41—C40—H40A	109.7
C1—C2—H2	120.0	S2—C40—H40A	109.7
C3—C2—H2	120.0	C41—C40—H40B	109.7
C4—C3—C2	119.08 (17)	S2—C40—H40B	109.7
C4—C3—H3	120.5	H40A—C40—H40B	108.2
C2—C3—H3	120.5	O4—C41—N9	121.41 (16)
C5—C4—C3	121.18 (16)	O4—C41—C40	123.20 (15)
C5—C4—Cl1	119.16 (14)	N9—C41—C40	115.37 (14)
C3—C4—Cl1	119.65 (14)	N10—C42—C43	120.19 (16)
C4—C5—C6	119.85 (16)	N10—C42—H42	119.9
C4—C5—H5	120.1	C43—C42—H42	119.9
C6—C5—H5	120.1	C44—C43—C48	119.28 (17)
C1—C6—C5	119.04 (15)	C44—C43—C42	119.05 (17)
C1—C6—H6	120.5	C48—C43—C42	121.66 (15)
C5—C6—H6	120.5	C45—C44—C43	120.23 (18)
O1—C7—C8	106.34 (13)	C45—C44—H44	119.9
O1—C7—H7A	110.5	C43—C44—H44	119.9
C8—C7—H7A	110.5	C46—C45—C44	120.10 (18)
O1—C7—H7B	110.5	C46—C45—H45	120.0
C8—C7—H7B	110.5	C44—C45—H45	120.0
H7A—C7—H7B	108.7	C45—C46—C47	120.19 (19)
N1—C8—N3	110.01 (14)	C45—C46—H46	119.9
N1—C8—C7	125.92 (15)	C47—C46—H46	119.9
N3—C8—C7	124.01 (14)	C48—C47—C46	120.0 (2)
N2—C9—N3	110.92 (14)	C48—C47—H47	120.0
N2—C9—S1	127.74 (12)	C46—C47—H47	120.0
N3—C9—S1	121.30 (12)	C47—C48—C43	120.18 (17)
C11—C10—C15	121.80 (15)	C47—C48—H48	119.9
C11—C10—N3	118.07 (15)	C43—C48—H48	119.9
C15—C10—N3	120.13 (15)	C63—S3—C64	96.30 (8)
C10—C11—C12	119.01 (17)	C49—O5—C55	116.14 (13)
C10—C11—H11	120.5	C56—N11—N12	107.98 (13)
C12—C11—H11	120.5	C63—N12—N11	106.20 (14)
C13—C12—C11	120.10 (18)	C63—N13—C56	104.31 (14)
C13—C12—H12	119.9	C63—N13—C57	127.68 (14)
C11—C12—H12	119.9	C56—N13—C57	127.21 (14)
C12—C13—C14	120.12 (17)	C65—N14—N15	121.52 (15)
C12—C13—H13	119.9	C65—N14—H14N	118.5
C14—C13—H13	119.9	N15—N14—H14N	119.9
C13—C14—C15	120.43 (17)	C66—N15—N14	115.49 (15)

C13—C14—H14	119.8	O5—C49—C50	115.39 (15)
C15—C14—H14	119.8	O5—C49—C54	123.84 (15)
C10—C15—C14	118.53 (17)	C50—C49—C54	120.74 (16)
C10—C15—H15	120.7	C49—C50—C51	120.17 (17)
C14—C15—H15	120.7	C49—C50—H50	119.9
C17—C16—S1	109.05 (11)	C51—C50—H50	119.9
C17—C16—H16A	109.9	C52—C51—C50	119.02 (17)
S1—C16—H16A	109.9	C52—C51—H51	120.5
C17—C16—H16B	109.9	C50—C51—H51	120.5
S1—C16—H16B	109.9	C53—C52—C51	120.91 (17)
H16A—C16—H16B	108.3	C53—C52—Cl3	119.54 (14)
O2—C17—N4	121.56 (15)	C51—C52—Cl3	119.54 (14)
O2—C17—C16	122.23 (14)	C52—C53—C54	120.19 (16)
N4—C17—C16	116.19 (14)	C52—C53—H53	119.9
N5—C18—C19	120.97 (15)	C54—C53—H53	119.9
N5—C18—H18	119.5	C49—C54—C53	118.97 (16)
C19—C18—H18	119.5	C49—C54—H54	120.5
C20—C19—C24	118.65 (15)	C53—C54—H54	120.5
C20—C19—C18	122.22 (15)	O5—C55—C56	107.07 (14)
C24—C19—C18	119.12 (15)	O5—C55—H55A	110.3
C21—C20—C19	120.39 (16)	C56—C55—H55A	110.3
C21—C20—H20	119.8	O5—C55—H55B	110.3
C19—C20—H20	119.8	C56—C55—H55B	110.3
C20—C21—C22	120.49 (19)	H55A—C55—H55B	108.6
C20—C21—H21	119.8	N11—C56—N13	110.27 (15)
C22—C21—H21	119.8	N11—C56—C55	125.53 (15)
C23—C22—C21	119.67 (18)	N13—C56—C55	124.16 (15)
C23—C22—H22	120.2	C62—C57—C58	121.49 (16)
C21—C22—H22	120.2	C62—C57—N13	120.12 (16)
C22—C23—C24	120.08 (16)	C58—C57—N13	118.38 (15)
C22—C23—H23	120.0	C57—C58—C59	119.32 (17)
C24—C23—H23	120.0	C57—C58—H58	120.3
C23—C24—C19	120.72 (17)	C59—C58—H58	120.3
C23—C24—H24	119.6	C60—C59—C58	119.82 (18)
C19—C24—H24	119.6	C60—C59—H59	120.1
C33—S2—C40	95.76 (8)	C58—C59—H59	120.1
C25—O3—C31	117.59 (13)	C61—C60—C59	120.24 (17)
C32—N6—N7	107.39 (13)	C61—C60—H60	119.9
C33—N7—N6	106.74 (13)	C59—C60—H60	119.9
C33—N8—C32	104.07 (13)	C60—C61—C62	120.61 (17)
C33—N8—C34	127.89 (14)	C60—C61—H61	119.7
C32—N8—C34	126.48 (14)	C62—C61—H61	119.7
C41—N9—N10	119.91 (14)	C57—C62—C61	118.52 (18)
C41—N9—H9N	118.8	C57—C62—H62	120.7
N10—N9—H9N	121.3	C61—C62—H62	120.7
C42—N10—N9	116.59 (15)	N12—C63—N13	111.24 (15)
O3—C25—C26	115.48 (15)	N12—C63—S3	127.30 (13)
O3—C25—C30	123.87 (15)	N13—C63—S3	121.45 (12)

C26—C25—C30	120.58 (16)	C65—C64—S3	109.11 (12)
C25—C26—C27	119.87 (18)	C65—C64—H64A	109.9
C25—C26—H26	120.1	S3—C64—H64A	109.9
C27—C26—H26	120.1	C65—C64—H64B	109.9
C28—C27—C26	119.45 (18)	S3—C64—H64B	109.9
C28—C27—H27	120.3	H64A—C64—H64B	108.3
C26—C27—H27	120.3	O6—C65—N14	121.07 (16)
C27—C28—C29	120.95 (17)	O6—C65—C64	121.71 (16)
C27—C28—Cl2	119.41 (14)	N14—C65—C64	117.20 (15)
C29—C28—Cl2	119.63 (14)	N15—C66—C67	121.05 (16)
C28—C29—C30	119.91 (17)	N15—C66—H66	119.5
C28—C29—H29	120.0	C67—C66—H66	119.5
C30—C29—H29	120.0	C72—C67—C68	118.78 (17)
C25—C30—C29	119.25 (16)	C72—C67—C66	122.41 (16)
C25—C30—H30	120.4	C68—C67—C66	118.80 (17)
C29—C30—H30	120.4	C69—C68—C67	120.40 (18)
O3—C31—C32	106.23 (13)	C69—C68—H68	119.8
O3—C31—H31A	110.5	C67—C68—H68	119.8
C32—C31—H31A	110.5	C70—C69—C68	120.16 (17)
O3—C31—H31B	110.5	C70—C69—H69	119.9
C32—C31—H31B	110.5	C68—C69—H69	119.9
H31A—C31—H31B	108.7	C69—C70—C71	119.94 (18)
N6—C32—N8	110.78 (14)	C69—C70—H70	120.0
N6—C32—C31	125.66 (15)	C71—C70—H70	120.0
N8—C32—C31	123.47 (14)	C72—C71—C70	120.17 (19)
N7—C33—N8	111.01 (14)	C72—C71—H71	119.9
N7—C33—S2	127.73 (12)	C70—C71—H71	119.9
N8—C33—S2	121.22 (12)	C71—C72—C67	120.54 (17)
C35—C34—C39	121.82 (15)	C71—C72—H72	119.7
C35—C34—N8	120.27 (15)	C67—C72—H72	119.7
C39—C34—N8	117.91 (14)	H7D—O7—H7C	104.1
C34—C35—C36	118.33 (17)	O8^{i}—O8—H8A	60.2
C34—C35—H35	120.8	H8A—O8—H8B	104.0

C8—N1—N2—C9	−0.56 (18)	C40—S2—C33—N8	−170.39 (14)
C17—N4—N5—C18	176.79 (15)	C33—N8—C34—C35	−87.0 (2)
C7—O1—C1—C2	149.15 (16)	C32—N8—C34—C35	109.6 (2)
C7—O1—C1—C6	−33.2 (2)	C33—N8—C34—C39	93.7 (2)
O1—C1—C2—C3	177.38 (18)	C32—N8—C34—C39	−69.7 (2)
C6—C1—C2—C3	−0.4 (3)	C39—C34—C35—C36	1.3 (3)
C1—C2—C3—C4	−0.1 (3)	N8—C34—C35—C36	−178.00 (16)
C2—C3—C4—C5	0.2 (3)	C34—C35—C36—C37	0.4 (3)
C2—C3—C4—Cl1	179.51 (16)	C35—C36—C37—C38	−1.5 (3)
C3—C4—C5—C6	0.3 (3)	C36—C37—C38—C39	0.9 (3)
Cl1—C4—C5—C6	−179.07 (13)	C35—C34—C39—C38	−1.8 (3)
C2—C1—C6—C5	0.8 (3)	N8—C34—C39—C38	177.46 (17)
O1—C1—C6—C5	−176.77 (15)	C37—C38—C39—C34	0.7 (3)
C4—C5—C6—C1	−0.8 (3)	C33—S2—C40—C41	176.14 (13)

C1—O1—C7—C8	−171.47 (13)	N10—N9—C41—O4	179.24 (15)
N2—N1—C8—N3	0.18 (18)	N10—N9—C41—C40	0.9 (2)
N2—N1—C8—C7	177.31 (15)	S2—C40—C41—O4	9.7 (2)
C9—N3—C8—N1	0.24 (18)	S2—C40—C41—N9	−172.01 (13)
C10—N3—C8—N1	−168.91 (15)	N9—N10—C42—C43	−179.38 (15)
C9—N3—C8—C7	−176.95 (15)	N10—C42—C43—C44	173.62 (17)
C10—N3—C8—C7	13.9 (3)	N10—C42—C43—C48	−5.2 (3)
O1—C7—C8—N1	−120.09 (17)	C48—C43—C44—C45	0.7 (3)
O1—C7—C8—N3	56.6 (2)	C42—C43—C44—C45	−178.18 (17)
N1—N2—C9—N3	0.73 (18)	C43—C44—C45—C46	−1.2 (3)
N1—N2—C9—S1	−177.01 (12)	C44—C45—C46—C47	0.8 (3)
C8—N3—C9—N2	−0.61 (18)	C45—C46—C47—C48	0.2 (4)
C10—N3—C9—N2	168.36 (15)	C46—C47—C48—C43	−0.7 (3)
C8—N3—C9—S1	177.29 (12)	C44—C43—C48—C47	0.3 (3)
C10—N3—C9—S1	−13.7 (2)	C42—C43—C48—C47	179.09 (18)
C16—S1—C9—N2	−7.22 (17)	C56—N11—N12—C63	0.71 (19)
C16—S1—C9—N3	175.25 (14)	C65—N14—N15—C66	−176.10 (16)
C9—N3—C10—C11	−101.6 (2)	C55—O5—C49—C50	−158.03 (16)
C8—N3—C10—C11	65.1 (2)	C55—O5—C49—C54	23.8 (2)
C9—N3—C10—C15	77.8 (2)	O5—C49—C50—C51	−178.40 (18)
C8—N3—C10—C15	−115.58 (19)	C54—C49—C50—C51	−0.2 (3)
C15—C10—C11—C12	0.7 (3)	C49—C50—C51—C52	0.5 (3)
N3—C10—C11—C12	−179.99 (17)	C50—C51—C52—C53	−0.1 (3)
C10—C11—C12—C13	−0.6 (3)	C50—C51—C52—Cl3	−179.50 (16)
C11—C12—C13—C14	0.0 (3)	C51—C52—C53—C54	−0.5 (3)
C12—C13—C14—C15	0.4 (3)	Cl3—C52—C53—C54	178.92 (13)
C11—C10—C15—C14	−0.3 (3)	O5—C49—C54—C53	177.66 (16)
N3—C10—C15—C14	−179.58 (16)	C50—C49—C54—C53	−0.4 (3)
C13—C14—C15—C10	−0.3 (3)	C52—C53—C54—C49	0.7 (3)
C9—S1—C16—C17	177.06 (13)	C49—O5—C55—C56	171.56 (14)
N5—N4—C17—O2	177.84 (14)	N12—N11—C56—N13	−0.38 (19)
N5—N4—C17—C16	−4.0 (2)	N12—N11—C56—C55	−177.96 (16)
S1—C16—C17—O2	−11.9 (2)	C63—N13—C56—N11	−0.09 (19)
S1—C16—C17—N4	169.94 (12)	C57—N13—C56—N11	170.26 (15)
N4—N5—C18—C19	179.70 (14)	C63—N13—C56—C55	177.53 (16)
N5—C18—C19—C20	5.5 (3)	C57—N13—C56—C55	−12.1 (3)
N5—C18—C19—C24	−173.33 (16)	O5—C55—C56—N11	122.18 (18)
C24—C19—C20—C21	0.4 (3)	O5—C55—C56—N13	−55.1 (2)
C18—C19—C20—C21	−178.38 (18)	C63—N13—C57—C62	−71.9 (2)
C19—C20—C21—C22	0.0 (3)	C56—N13—C57—C62	119.97 (19)
C20—C21—C22—C23	−0.3 (3)	C63—N13—C57—C58	107.1 (2)
C21—C22—C23—C24	0.3 (3)	C56—N13—C57—C58	−61.1 (2)
C22—C23—C24—C19	0.1 (3)	C62—C57—C58—C59	0.5 (3)
C20—C19—C24—C23	−0.5 (3)	N13—C57—C58—C59	−178.39 (16)
C18—C19—C24—C23	178.37 (16)	C57—C58—C59—C60	0.2 (3)
C32—N6—N7—C33	0.63 (17)	C58—C59—C60—C61	−0.8 (3)
C41—N9—N10—C42	−176.21 (16)	C59—C60—C61—C62	0.6 (3)
C31—O3—C25—C26	−149.29 (17)	C58—C57—C62—C61	−0.7 (3)

C31—O3—C25—C30	33.8 (2)	N13—C57—C62—C61	178.18 (16)
O3—C25—C26—C27	−176.77 (19)	C60—C61—C62—C57	0.2 (3)
C30—C25—C26—C27	0.2 (3)	N11—N12—C63—N13	−0.79 (19)
C25—C26—C27—C28	−0.1 (3)	N11—N12—C63—S3	178.29 (13)
C26—C27—C28—C29	0.2 (3)	C56—N13—C63—N12	0.56 (19)
C26—C27—C28—Cl2	−178.96 (17)	C57—N13—C63—N12	−169.72 (16)
C27—C28—C29—C30	−0.4 (3)	C56—N13—C63—S3	−178.58 (12)
Cl2—C28—C29—C30	178.75 (14)	C57—N13—C63—S3	11.1 (2)
O3—C25—C30—C29	176.29 (16)	C64—S3—C63—N12	−3.31 (18)
C26—C25—C30—C29	−0.4 (3)	C64—S3—C63—N13	175.68 (15)
C28—C29—C30—C25	0.5 (3)	C63—S3—C64—C65	176.38 (13)
C25—O3—C31—C32	176.58 (14)	N15—N14—C65—O6	−177.96 (16)
N7—N6—C32—N8	−0.41 (18)	N15—N14—C65—C64	3.5 (2)
N7—N6—C32—C31	−177.17 (15)	S3—C64—C65—O6	23.7 (2)
C33—N8—C32—N6	0.04 (18)	S3—C64—C65—N14	−157.77 (13)
C34—N8—C32—N6	166.64 (15)	N14—N15—C66—C67	−179.26 (15)
C33—N8—C32—C31	176.89 (15)	N15—C66—C67—C72	−2.7 (3)
C34—N8—C32—C31	−16.5 (3)	N15—C66—C67—C68	176.14 (17)
O3—C31—C32—N6	119.30 (17)	C72—C67—C68—C69	0.6 (3)
O3—C31—C32—N8	−57.1 (2)	C66—C67—C68—C69	−178.20 (17)
N6—N7—C33—N8	−0.62 (18)	C67—C68—C69—C70	−0.5 (3)
N6—N7—C33—S2	177.23 (12)	C68—C69—C70—C71	−0.1 (3)
C32—N8—C33—N7	0.38 (18)	C69—C70—C71—C72	0.5 (3)
C34—N8—C33—N7	−165.96 (15)	C70—C71—C72—C67	−0.3 (3)
C32—N8—C33—S2	−177.63 (12)	C68—C67—C72—C71	−0.2 (3)
C34—N8—C33—S2	16.0 (2)	C66—C67—C72—C71	178.56 (18)
C40—S2—C33—N7	11.95 (17)		

Symmetry code: (i) $-x, -y+1, -z$.

Hydrogen-bond geometry (Å, º)

Cg1 and Cg9 are the centroids of the 1,2,4-triazole rings N1–N3/C8/C9 and N11–N13/C56/C63, Cg2 and Cg10 are the centroids of the chlorophenyl rings C1–C6 and C49–C54, and Cg4 and Cg12 are the centroids of the phenyl rings C19–C24 and C67–C72.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4*N*···O7^{ii}	0.91	1.86	2.7527 (19)	166
C6—H6···O2^{iii}	0.95	2.36	3.2815 (19)	163
C7—H7*A*···O2^{iii}	0.99	2.35	3.304 (2)	162
C30—H30···O4^{ii}	0.95	2.48	3.395 (2)	161
C31—H31*B*···O4^{ii}	0.99	2.44	3.419 (2)	170
C39—H39···N6^{iv}	0.95	2.51	3.386 (2)	154
N14—H14*N*···O8	0.91	1.98	2.802 (3)	149
C54—H54···O6^{ii}	0.95	2.41	3.329 (2)	163
C55—H55*B*···O6^{ii}	0.99	2.35	3.254 (2)	151
O7—H7*D*···O4^{ii}	0.87	2.14	2.9668 (19)	160
O7—H7*C*···N1	0.87	1.96	2.8239 (19)	176
O8—H8*A*···N11^{iii}	0.87	2.05	2.897 (3)	164
O8—H8*B*···N11^{v}	0.87	2.16	2.853 (3)	136

C15—H15···*Cg*8^{ii}	0.95	2.74	3.670 (2)	168
C35—H35···*Cg*4^{iii}	0.95	2.77	3.709 (2)	169
C62—H62···*Cg*12^{v}	0.95	2.81	3.714 (2)	159

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