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1-(4-Methylphenyl)-3-phenyl-1*H*-pyrazol-5-yl 4-nitrobenzenesulfonate

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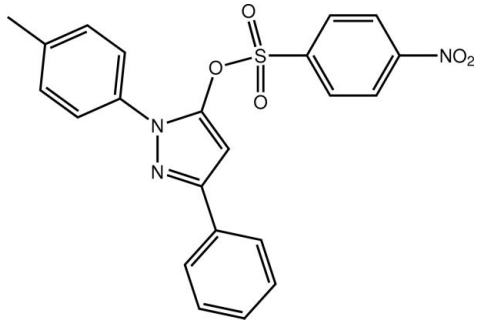
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.006 Å; R factor = 0.069; wR factor = 0.179; data-to-parameter ratio = 15.8.

In the title molecule, $C_{22}H_{17}N_3O_5S$, the pyrazole ring is planar (r.m.s. deviation = 0.018 Å) and forms dihedral angles of 21.45 (10) and 6.96 (10)° with the N- and C-bound benzene rings, respectively. Supramolecular layers in the *bc* plane are formed in the crystal *via* C—H···O and π–π interactions involving the sulfonamide benzene ring interacting with the N- and C-bound benzene rings [centroid–centroid distances = 3.790 (2) and 3.730 (2) Å, respectively]. The crystal studied was found to be a merohedral twin (twin law 1 0 0.678, 0 $\overline{1}$ 0, 0 0 $\overline{1}$), the fractional contribution of the minor component being approximately 36%.

Related literature

For related structures and background references to pyrazoles, see: Wardell *et al.* (2012); Baddeley *et al.* (2012). For the synthesis, see: Galoyan *et al.* (1969). For the treatment of twinned diffraction data, see: Spek (2009).



Experimental

Crystal data

$C_{22}H_{17}N_3O_5S$
M_r = 435.46
Monoclinic, $P2_1/c$
a = 13.5339 (12) Å
b = 10.4827 (10) Å
c = 14.9303 (13) Å
β = 111.975 (3)°
V = 1964.3 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 120 K
0.58 × 0.38 × 0.04 mm

Data collection

Rigaku Saturn724+ diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
T_{min} = 0.620, T_{max} = 0.746
4454 measured reflections
4454 independent reflections
3951 reflections with $I > 2\sigma(I)$

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.179
S = 1.19
4454 reflections
282 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.62 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O4^{i}	0.95	2.50	3.387 (5)	155

Symmetry code: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6674).

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supplementary materials

Acta Cryst. (2012). E**68**, o1086–o1087 [doi:10.1107/S1600536812010598]

1-(4-Methylphenyl)-3-phenyl-1*H*-pyrazol-5-yl 4-nitrobenzenesulfonate

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Comment

The structure of the title compound is now reported in continuation of related structural studies (Wardell *et al.* 2012; Baddeley *et al.*, 2012).

In the title compound, Fig. 2, the pyrazole ring is planar with a r.m.s. deviation for the fitted atoms of 0.018 Å; the maximum deviations from this plane are 0.015 (1) Å (for the N1 atom) and -0.015 (1) Å (C8). The N– and C-bound benzene rings are inclined to this plane forming dihedral angles of 21.45 (10) and 6.96 (10)°, respectively; the dihedral angle between the benzene rings is 20.42 (10)° consistent with a non-planar molecule.

In the crystal, molecules are assembled into supramolecular layers in the *bc* plane *via* C—H···O, Table 1, and *π*—*π* interactions involving the sulfonamide benzene ring interacting with the N– and C-bound benzene rings {ring centroid···ring centroid distances = 3.790 (2) Å [angle of inclination = 0.96 (17)° for symmetry operation 1 - *x*, 1 - *y*, -*z*] and 3.730 (2) Å [angle of inclination = 10.02 (17)° for symmetry operation 1 - *x*, -1/2 + *y*, -1/2 - *z*], respectively}, Fig. 3. Layers stack along the *a* axis with no specific interactions between them, Fig. 4.

Experimental

A solution of 4-Me$C_6H_4NHNH_2$.HCl (2 mmol) and $PhCOCH_2CONHPh$ (2 mmol) in Me_2CO (20 ml) was refluxed for 1 h. A solution of 4-nitrobenzenesulfonyl chloride (2 mmol) in Me_2CO (10 ml) was added and the reaction mixture was refluxed for 30 min, rotary evaporated and the residue was recrystallized twice from EtOH as yellow plates, *M*.pt: 445–447 K.

Refinement

The C-bound H atoms were geometrically placed (C—H = 0.95–0.98 Å) and refined as riding with U_{iso}(H) = 1.2–1.5U_{eq}(C). Owing to poor agreement three reflections, *i.e.* ($\bar{7}$ 0 10), ($\bar{7}$ 1 13) and ($\bar{1}$2 5 13), were removed from the final cycles of refinement. The sample was a non-merohedral twin (twin law 1 0 0.678, 0 $\bar{1}$ 0, 0 0 $\bar{1}$) and the fractional contribution of the minor component refined to 0.362 (2). The twin domains were separated by using the *TwinRotMat* routine in *PLATON* (Spek, 2009).

Computing details

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

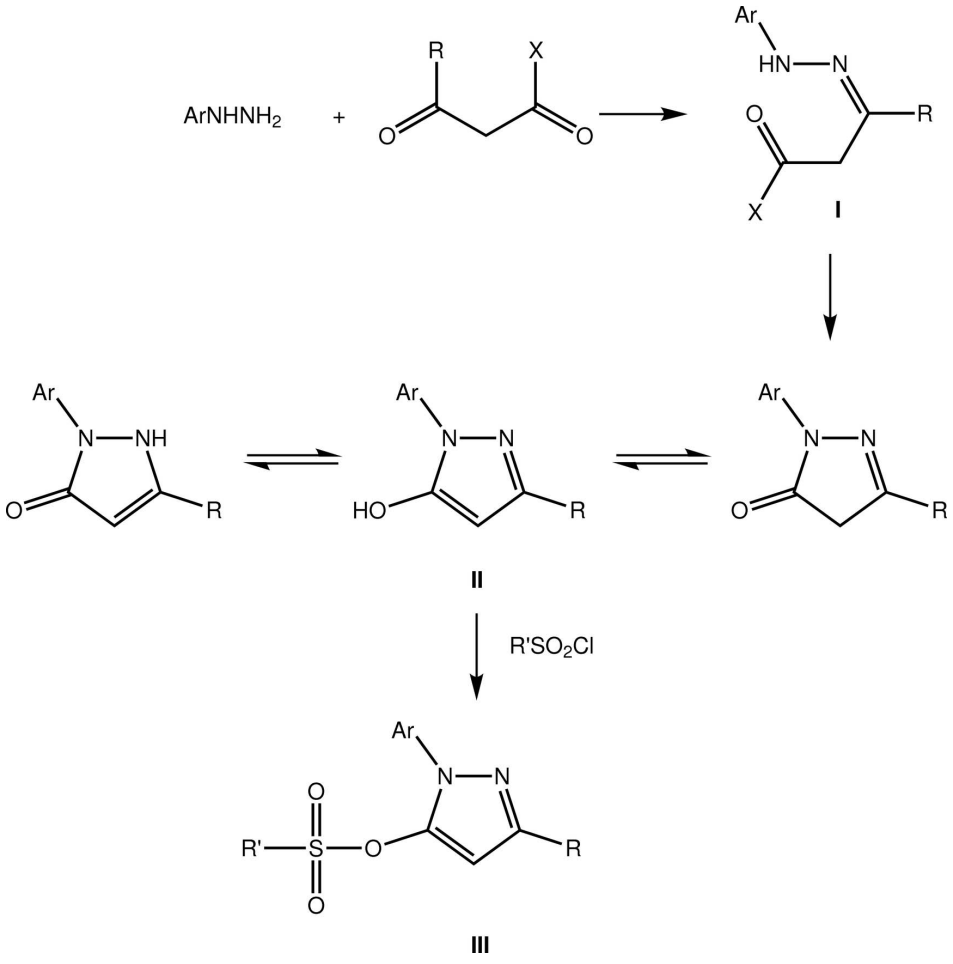

Figure 1

Reaction scheme. For further details see Baddeley *et al.* (2012).

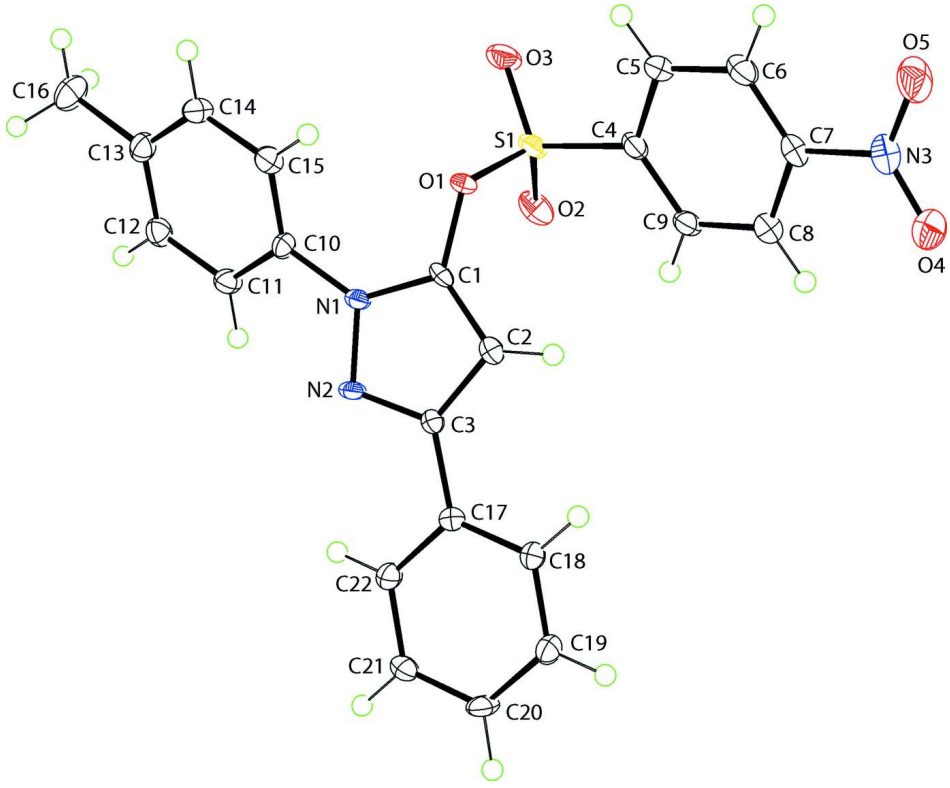

Figure 2

The molecular structure of (I) showing displacement ellipsoids at the 50% probability level.

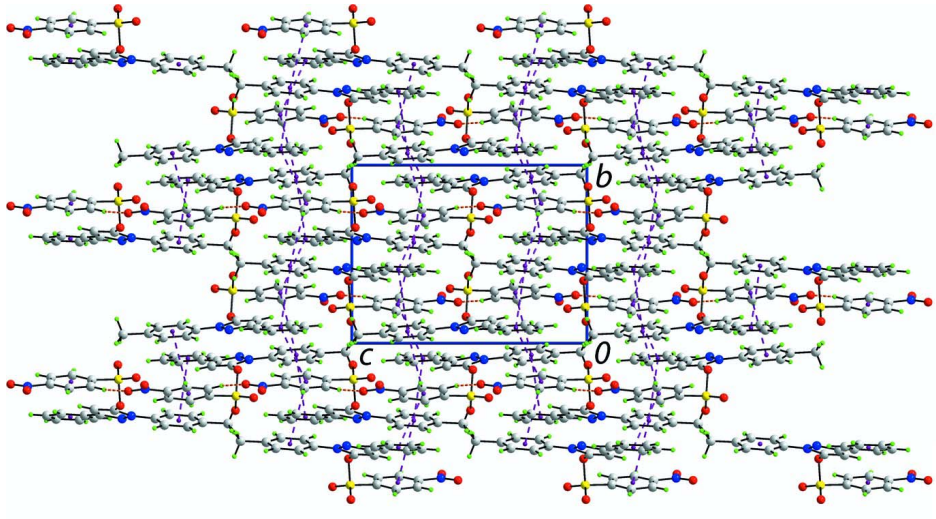

Figure 3

Supramolecular layer in the *bc* plane in (I) sustained by C—H···O and π—π interactions shown as orange and purple dashed lines, respectively.

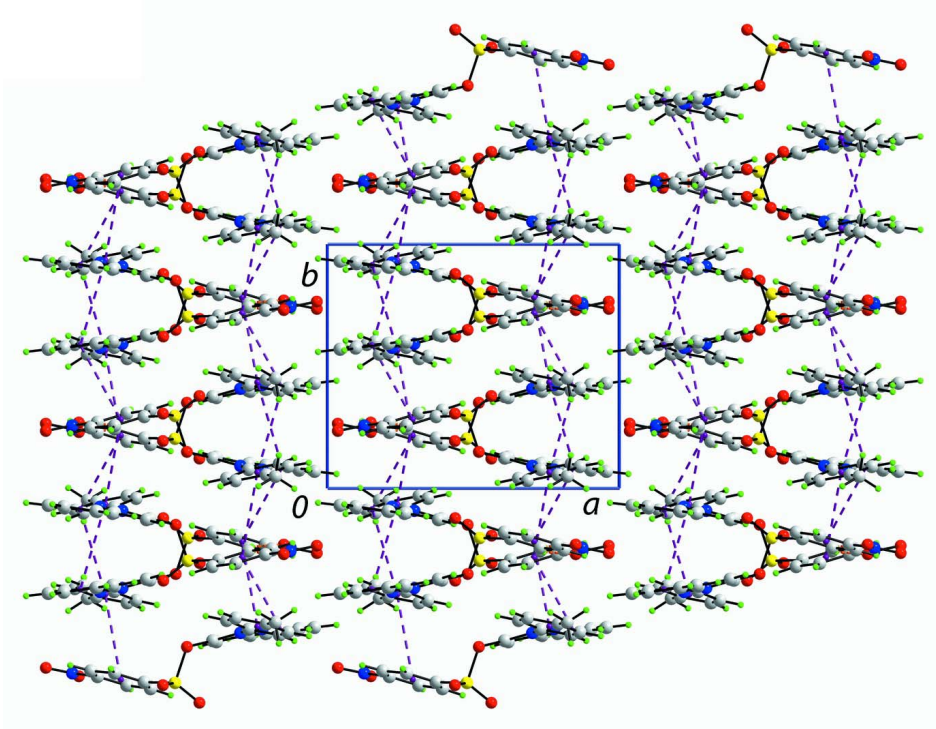

Figure 4

A view in projection down the *c* axis of the crystal packing in (I) showing the stacking of layers. The C—H···O, and π—π interactions are shown as orange and purple dashed lines, respectively.

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Crystal data

$C_{22}H_{17}N_3O_5S$
$M_r = 435.46$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 13.5339\ (12)$ Å
$b = 10.4827\ (10)$ Å
$c = 14.9303\ (13)$ Å
$\beta = 111.975\ (3)°$
$V = 1964.3\ (3)$ Å^3
$Z = 4$
$F(000) = 904$
$D_x = 1.472$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 67707 reflections
$\theta = 2.9–27.5°$
$\mu = 0.21$ mm^{-1}
$T = 120$ K
Plate, yellow
0.58 × 0.38 × 0.04 mm

Data collection

Rigaku Saturn724+ diffractometer
Radiation source: Rotating Anode
Confocal monochromator
Detector resolution: 28.5714 pixels mm^{-1}
profile data from ω–scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
$T_{min} = 0.620$, $T_{max} = 0.746$
4454 measured reflections
4454 independent reflections
3951 reflections with $I > 2\sigma(I)$
$R_{int} = 0.000$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.2°$
$h = -17\rightarrow16$
$k = 0\rightarrow13$
$l = 0\rightarrow19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.069$
$wR(F^2) = 0.179$
$S = 1.19$
4454 reflections
282 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0562P)^2 + 4.737P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.59$ e Å^{-3}
$\Delta\rho_{min} = -0.62$ e Å^{-3}

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.47829 (6)	0.20331 (9)	0.00726 (6)	0.0203 (2)
O1	0.51909 (18)	0.3508 (3)	0.01445 (17)	0.0203 (5)
O2	0.5619 (2)	0.1219 (3)	0.0044 (2)	0.0268 (6)
O3	0.4369 (2)	0.1938 (3)	0.08223 (19)	0.0315 (7)
O4	0.1490 (2)	0.2303 (3)	−0.4513 (2)	0.0360 (7)
O5	0.0359 (2)	0.2650 (3)	−0.3824 (2)	0.0377 (8)
N1	0.7023 (2)	0.4081 (3)	0.0618 (2)	0.0156 (6)
N2	0.7780 (2)	0.4243 (3)	0.0225 (2)	0.0156 (6)
N3	0.1265 (2)	0.2427 (3)	−0.3796 (2)	0.0254 (7)
C1	0.6074 (2)	0.3760 (3)	−0.0095 (2)	0.0169 (7)
C2	0.7290 (2)	0.4006 (3)	−0.0717 (2)	0.0141 (6)
C3	0.6198 (3)	0.3718 (3)	−0.0957 (2)	0.0183 (7)
H3	0.5673	0.3539	−0.1576	0.022*
C4	0.3726 (3)	0.2062 (3)	−0.1065 (3)	0.0185 (7)
C5	0.2715 (3)	0.2430 (4)	−0.1110 (3)	0.0206 (7)
H5	0.2587	0.2609	−0.0539	0.025*
C6	0.1898 (3)	0.2525 (4)	−0.2022 (3)	0.0222 (7)
H6	0.1196	0.2749	−0.2081	0.027*
C7	0.2126 (3)	0.2292 (3)	−0.2831 (3)	0.0199 (7)
C8	0.3132 (3)	0.1929 (4)	−0.2796 (3)	0.0220 (7)
H8	0.3262	0.1777	−0.3370	0.026*
C9	0.3942 (3)	0.1796 (3)	−0.1886 (3)	0.0189 (7)
H9	0.4633	0.1527	−0.1829	0.023*
C10	0.7302 (3)	0.4228 (3)	0.1639 (2)	0.0152 (6)
C11	0.8359 (3)	0.3992 (3)	0.2245 (3)	0.0181 (7)
H11	0.8871	0.3757	0.1980	0.022*

C12	0.8651 (3)	0.4106 (3)	0.3239 (2)	0.0198 (7)
H12	0.9369	0.3951	0.3651	0.024*
C13	0.7909 (3)	0.4445 (3)	0.3644 (3)	0.0210 (7)
C14	0.6856 (3)	0.4686 (4)	0.3023 (3)	0.0211 (7)
H14	0.6343	0.4919	0.3287	0.025*
C15	0.6551 (3)	0.4590 (3)	0.2020 (3)	0.0197 (7)
H15	0.5838	0.4770	0.1604	0.024*
C16	0.8218 (3)	0.4510 (4)	0.4733 (3)	0.0307 (9)
H16A	0.7642	0.4912	0.4879	0.046*
H16B	0.8871	0.5014	0.5020	0.046*
H16C	0.8341	0.3645	0.5002	0.046*
C17	0.7883 (3)	0.4054 (3)	−0.1369 (2)	0.0157 (6)
C18	0.7359 (3)	0.3973 (3)	−0.2370 (2)	0.0166 (6)
H18	0.6609	0.3851	−0.2640	0.020*
C19	0.7925 (3)	0.4068 (3)	−0.2978 (2)	0.0191 (7)
H19	0.7563	0.4007	−0.3658	0.023*
C20	0.9031 (3)	0.4255 (4)	−0.2584 (3)	0.0210 (7)
H20	0.9417	0.4348	−0.2997	0.025*
C21	0.9563 (3)	0.4303 (3)	−0.1586 (3)	0.0194 (7)
H21	1.0315	0.4409	−0.1319	0.023*
C22	0.8997 (3)	0.4196 (3)	−0.0977 (2)	0.0185 (7)
H22	0.9365	0.4218	−0.0297	0.022*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0124 (4)	0.0288 (5)	0.0195 (4)	−0.0052 (3)	0.0057 (3)	0.0020 (4)
O1	0.0110 (10)	0.0319 (14)	0.0212 (12)	−0.0056 (10)	0.0097 (10)	−0.0077 (10)
O2	0.0167 (12)	0.0245 (14)	0.0359 (15)	0.0004 (10)	0.0058 (11)	0.0053 (12)
O3	0.0206 (12)	0.0545 (19)	0.0206 (13)	−0.0108 (13)	0.0090 (11)	0.0067 (13)
O4	0.0335 (15)	0.0501 (19)	0.0210 (14)	−0.0070 (14)	0.0061 (12)	−0.0007 (13)
O5	0.0202 (13)	0.050 (2)	0.0338 (16)	0.0089 (13)	−0.0002 (12)	−0.0092 (14)
N1	0.0106 (12)	0.0238 (15)	0.0136 (13)	−0.0030 (11)	0.0057 (11)	0.0008 (11)
N2	0.0110 (12)	0.0238 (15)	0.0144 (13)	−0.0021 (11)	0.0075 (11)	0.0014 (11)
N3	0.0230 (15)	0.0232 (16)	0.0244 (17)	−0.0028 (13)	0.0024 (13)	−0.0025 (13)
C1	0.0077 (13)	0.0240 (17)	0.0179 (15)	−0.0046 (12)	0.0034 (12)	−0.0022 (14)
C2	0.0113 (14)	0.0175 (16)	0.0127 (15)	−0.0014 (12)	0.0034 (12)	−0.0004 (12)
C3	0.0126 (14)	0.0237 (18)	0.0171 (16)	−0.0034 (13)	0.0037 (12)	−0.0022 (13)
C4	0.0124 (14)	0.0224 (17)	0.0190 (16)	−0.0046 (13)	0.0040 (12)	−0.0001 (14)
C5	0.0161 (15)	0.0254 (18)	0.0228 (18)	−0.0043 (14)	0.0100 (13)	−0.0032 (14)
C6	0.0139 (15)	0.0242 (18)	0.0274 (19)	−0.0010 (14)	0.0066 (14)	−0.0014 (15)
C7	0.0146 (15)	0.0196 (17)	0.0225 (17)	−0.0042 (13)	0.0035 (13)	−0.0020 (14)
C8	0.0190 (16)	0.0241 (18)	0.0227 (17)	−0.0044 (14)	0.0077 (14)	−0.0029 (14)
C9	0.0137 (14)	0.0210 (17)	0.0240 (18)	−0.0029 (13)	0.0093 (13)	−0.0036 (14)
C10	0.0163 (15)	0.0177 (16)	0.0104 (15)	−0.0014 (12)	0.0036 (12)	−0.0001 (12)
C11	0.0141 (15)	0.0231 (17)	0.0172 (16)	0.0001 (13)	0.0060 (13)	0.0017 (13)
C12	0.0174 (16)	0.0220 (18)	0.0172 (17)	−0.0024 (13)	0.0034 (13)	0.0007 (13)
C13	0.0273 (18)	0.0200 (17)	0.0164 (16)	−0.0054 (14)	0.0090 (14)	−0.0015 (14)
C14	0.0214 (17)	0.0235 (18)	0.0225 (18)	−0.0019 (14)	0.0130 (15)	−0.0020 (14)
C15	0.0170 (15)	0.0209 (16)	0.0218 (17)	−0.0019 (13)	0.0080 (14)	−0.0015 (14)

C16	0.037 (2)	0.039 (2)	0.0143 (17)	−0.0007 (18)	0.0082 (16)	0.0005 (16)
C17	0.0159 (15)	0.0178 (16)	0.0145 (15)	−0.0020 (12)	0.0071 (13)	−0.0001 (12)
C18	0.0159 (15)	0.0189 (16)	0.0137 (15)	−0.0007 (12)	0.0040 (12)	−0.0002 (13)
C19	0.0209 (16)	0.0214 (17)	0.0135 (16)	−0.0014 (13)	0.0050 (13)	−0.0006 (13)
C20	0.0217 (17)	0.0263 (19)	0.0220 (18)	−0.0007 (14)	0.0163 (15)	−0.0008 (14)
C21	0.0134 (15)	0.0246 (18)	0.0207 (17)	−0.0030 (13)	0.0071 (13)	−0.0002 (14)
C22	0.0161 (15)	0.0248 (18)	0.0135 (15)	−0.0007 (13)	0.0045 (13)	−0.0001 (13)

Geometric parameters (Å, º)

S1—O3	1.430 (3)	C10—C15	1.391 (5)
S1—O2	1.431 (3)	C10—C11	1.399 (4)
S1—O1	1.632 (3)	C11—C12	1.391 (5)
S1—C4	1.765 (3)	C11—H11	0.9500
O1—C1	1.395 (4)	C12—C13	1.397 (5)
O4—N3	1.225 (4)	C12—H12	0.9500
O5—N3	1.233 (4)	C13—C14	1.402 (5)
N1—N2	1.366 (4)	C13—C16	1.522 (5)
N1—C1	1.368 (4)	C14—C15	1.401 (5)
N1—C10	1.435 (4)	C14—H14	0.9500
N2—C2	1.336 (4)	C15—H15	0.9500
N3—C7	1.482 (5)	C16—H16A	0.9800
C1—C3	1.360 (5)	C16—H16B	0.9800
C2—C3	1.417 (4)	C16—H16C	0.9800
C2—C17	1.476 (4)	C17—C18	1.397 (5)
C3—H3	0.9500	C17—C22	1.406 (5)
C4—C9	1.390 (5)	C18—C19	1.393 (5)
C4—C5	1.399 (5)	C18—H18	0.9500
C5—C6	1.399 (5)	C19—C20	1.402 (5)
C5—H5	0.9500	C19—H19	0.9500
C6—C7	1.376 (5)	C20—C21	1.391 (5)
C6—H6	0.9500	C20—H20	0.9500
C7—C8	1.396 (5)	C21—C22	1.396 (5)
C8—C9	1.397 (5)	C21—H21	0.9500
C8—H8	0.9500	C22—H22	0.9500
C9—H9	0.9500		

O3—S1—O2	121.83 (18)	C15—C10—N1	121.5 (3)
O3—S1—O1	103.66 (16)	C11—C10—N1	117.8 (3)
O2—S1—O1	108.38 (14)	C12—C11—C10	119.2 (3)
O3—S1—C4	109.94 (16)	C12—C11—H11	120.4
O2—S1—C4	110.29 (17)	C10—C11—H11	120.4
O1—S1—C4	100.35 (15)	C11—C12—C13	121.4 (3)
C1—O1—S1	117.6 (2)	C11—C12—H12	119.3
N2—N1—C1	109.5 (3)	C13—C12—H12	119.3
N2—N1—C10	120.0 (3)	C12—C13—C14	118.5 (3)
C1—N1—C10	130.5 (3)	C12—C13—C16	121.3 (3)
C2—N2—N1	105.8 (2)	C14—C13—C16	120.2 (3)
O4—N3—O5	124.0 (3)	C15—C14—C13	120.9 (3)
O4—N3—C7	118.5 (3)	C15—C14—H14	119.5

O5—N3—C7	117.4 (3)	C13—C14—H14	119.5
C3—C1—N1	109.4 (3)	C10—C15—C14	119.2 (3)
C3—C1—O1	131.1 (3)	C10—C15—H15	120.4
N1—C1—O1	119.5 (3)	C14—C15—H15	120.4
N2—C2—C3	111.4 (3)	C13—C16—H16A	109.5
N2—C2—C17	120.7 (3)	C13—C16—H16B	109.5
C3—C2—C17	127.9 (3)	H16A—C16—H16B	109.5
C1—C3—C2	103.9 (3)	C13—C16—H16C	109.5
C1—C3—H3	128.0	H16A—C16—H16C	109.5
C2—C3—H3	128.0	H16B—C16—H16C	109.5
C9—C4—C5	122.5 (3)	C18—C17—C22	119.2 (3)
C9—C4—S1	118.9 (3)	C18—C17—C2	121.3 (3)
C5—C4—S1	118.5 (3)	C22—C17—C2	119.5 (3)
C4—C5—C6	118.0 (3)	C19—C18—C17	120.7 (3)
C4—C5—H5	121.0	C19—C18—H18	119.7
C6—C5—H5	121.0	C17—C18—H18	119.7
C7—C6—C5	119.1 (3)	C18—C19—C20	119.8 (3)
C7—C6—H6	120.4	C18—C19—H19	120.1
C5—C6—H6	120.4	C20—C19—H19	120.1
C6—C7—C8	123.5 (3)	C21—C20—C19	119.9 (3)
C6—C7—N3	118.9 (3)	C21—C20—H20	120.1
C8—C7—N3	117.6 (3)	C19—C20—H20	120.1
C7—C8—C9	117.5 (3)	C20—C21—C22	120.3 (3)
C7—C8—H8	121.2	C20—C21—H21	119.9
C9—C8—H8	121.2	C22—C21—H21	119.9
C4—C9—C8	119.4 (3)	C21—C22—C17	120.1 (3)
C4—C9—H9	120.3	C21—C22—H22	119.9
C8—C9—H9	120.3	C17—C22—H22	119.9
C15—C10—C11	120.7 (3)		

O3—S1—O1—C1	147.7 (2)	C6—C7—C8—C9	0.2 (6)
O2—S1—O1—C1	17.0 (3)	N3—C7—C8—C9	−179.7 (3)
C4—S1—O1—C1	−98.6 (2)	C5—C4—C9—C8	1.7 (5)
C1—N1—N2—C2	−0.7 (4)	S1—C4—C9—C8	−174.2 (3)
C10—N1—N2—C2	178.1 (3)	C7—C8—C9—C4	−1.8 (5)
N2—N1—C1—C3	−0.5 (4)	N2—N1—C10—C15	153.3 (3)
C10—N1—C1—C3	−179.1 (3)	C1—N1—C10—C15	−28.3 (6)
N2—N1—C1—O1	178.0 (3)	N2—N1—C10—C11	−26.9 (5)
C10—N1—C1—O1	−0.5 (6)	C1—N1—C10—C11	151.6 (4)
S1—O1—C1—C3	69.1 (5)	C15—C10—C11—C12	0.9 (5)
S1—O1—C1—N1	−109.1 (3)	N1—C10—C11—C12	−179.0 (3)
N1—N2—C2—C3	1.5 (4)	C10—C11—C12—C13	0.4 (5)
N1—N2—C2—C17	−178.1 (3)	C11—C12—C13—C14	−0.8 (5)
N1—C1—C3—C2	1.3 (4)	C11—C12—C13—C16	177.2 (4)
O1—C1—C3—C2	−177.0 (4)	C12—C13—C14—C15	0.1 (5)
N2—C2—C3—C1	−1.8 (4)	C16—C13—C14—C15	−177.9 (4)
C17—C2—C3—C1	177.8 (3)	C11—C10—C15—C14	−1.6 (5)
O3—S1—C4—C9	−162.3 (3)	N1—C10—C15—C14	178.2 (3)
O2—S1—C4—C9	−25.3 (3)	C13—C14—C15—C10	1.1 (5)

O1—S1—C4—C9	88.9 (3)	N2—C2—C17—C18	−171.6 (3)
O3—S1—C4—C5	21.6 (4)	C3—C2—C17—C18	8.8 (5)
O2—S1—C4—C5	158.7 (3)	N2—C2—C17—C22	7.8 (5)
O1—S1—C4—C5	−87.2 (3)	C3—C2—C17—C22	−171.8 (3)
C9—C4—C5—C6	0.2 (5)	C22—C17—C18—C19	−1.9 (5)
S1—C4—C5—C6	176.1 (3)	C2—C17—C18—C19	177.5 (3)
C4—C5—C6—C7	−1.8 (5)	C17—C18—C19—C20	−0.4 (5)
C5—C6—C7—C8	1.6 (6)	C18—C19—C20—C21	2.1 (6)
C5—C6—C7—N3	−178.4 (3)	C19—C20—C21—C22	−1.5 (6)
O4—N3—C7—C6	175.1 (4)	C20—C21—C22—C17	−0.8 (5)
O5—N3—C7—C6	−5.4 (5)	C18—C17—C22—C21	2.5 (5)
O4—N3—C7—C8	−5.0 (5)	C2—C17—C22—C21	−177.0 (3)
O5—N3—C7—C8	174.5 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O4^{i}	0.95	2.50	3.387 (5)	155

Symmetry code: (i) *x*, −*y*+1/2, *z*+1/2.