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(*E*)-2,4,6-Triisopropyl-*N*-[2-(2-pyridylmethyleneamino)cyclohexyl]benzenesulfonamide acetonitrile hemisolvate

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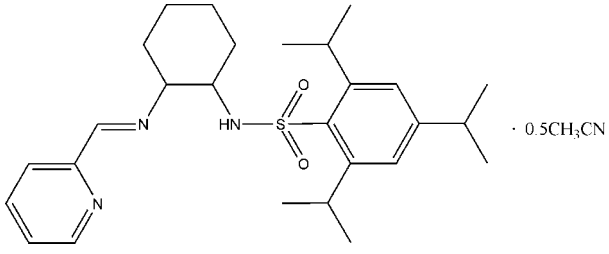
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; H-atom completeness 97%; R factor = 0.062; wR factor = 0.216; data-to-parameter ratio = 18.4.

The title compound, $C_{27}H_{39}N_3O_2S\cdot0.5CH_3CN$, a Schiff base ligand, was synthesized by the condensation of picolinaldehyde and *N*-(2-aminocyclohexyl)-2,4,6-triisopropylbenzenesulfonamide in ethanol. Crystals were grown from an acetonitrile solution. The cyclohexane ring has a chair conformation and the dihedral angle between the pyridine and benzene rings is 55.6°. The molecules form dimers *via* N—H···N hydrogen bonds.

Related literature

For related literature, see: Cabaret *et al.* (2004); Chamberlain *et al.* (1999); Endo *et al.* (1987).



Experimental

Crystal data

$C_{27}H_{39}N_3O_2S\cdot0.5C_2H_3N$
M_r = 488.70
Tetragonal, $I4_1/a$
a = 21.9895 (17) Å
c = 24.035 (3) Å
V = 11622.0 (18) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 0.14 mm^{-1}
T = 293 (2) K
0.30 × 0.28 × 0.20 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.769, T_{max} = 1.000
(expected range = 0.748–0.973)
31641 measured reflections
5766 independent reflections
3108 reflections with $I > 2\sigma(I)$
R_{int} = 0.063

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.216
S = 1.04
5766 reflections
313 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···N1^{i}	0.86	2.42	3.188 (4)	149

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

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ER2029).

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supplementary materials

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(*E*)-2,4,6-Triisopropyl-*N*-[2-(2-pyridylmethyleneamino)cyclohexyl]benzenesulfonamide acetonitrile hemisolvate

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Comment

In past two decade, significant advances have been made in polymerization of cyclic ester, such as poly(ε-caprolactone) (Endo *et al.*, 1987), poly(lactide) (Chamberlain *et al.*, 1999). The title compound (I), is designed as catalyst ligand for polymerization of poly(lactide). This ligand is one charge bulky shiff base after deprotonation, this kind of ligand is very useful in the ring-opening polymerization of cyclic esters (Cabaret *et al.*, 2004). In the present study, the bulky shiff base ligand derived from the condensation of picolinaldehyde and *N*-(2-aminocyclohexyl)-2,4,6-triisopropyl benzenesulfonamide in ethanol, was synthesized for the investigation of its application in the Ring-Opening polymerization of cyclic esters.

The geometric parameters for (I) are normal (Fig. 1). The compound is a dimer with an intermolecular N3—H3A–N1 hydrogen bond (Fig. 2).

Experimental

5.5 mmol picolinaldehyde was added to a solution of 5 mmol *N*-(2-aminocyclohexyl)-2,4,6-triisopropyl benzenesulfonamide in 30 ml e thanol. After stirring at room temperature for 4 h, the yellow precipitate was filtrated and washed with 10 ml e thanol. This compound was dried in vacuum and crystals grown from a solution of the title compound in acetonitrile.

Refinement

H atoms were placed in calculated positions and refined using a riding model, with d(N—H) = 0.86 Å and U_{iso}(H) = 1.2U_{eq}(N), d(C—H) = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for Csp^2, d(C—H) = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for the methylene groups, and d(C—H) = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for the methyl groups. The three H atoms of the acetonitrile solvate molecules were not located. The value of the Flack parameter is meaningless because of its large s.u. value thus the Friedel equivalents were merged in the final refinements.

Figures

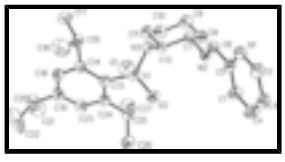

Fig. 1. Displacement ellipsoid plot.

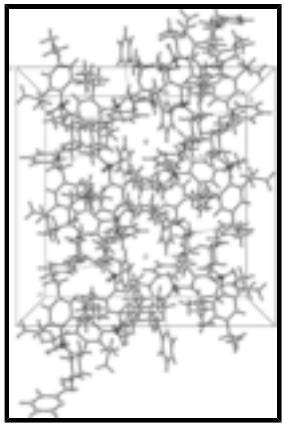

Fig. 2. Packing diagram.

(*E*)-2,4,6-Triisopropyl-N-[2- (2-pyridylmethyleneamino)cyclohexyl]benzenesulfonamide acetonitrile hemisolvate

Crystal data

$C_{27}H_{39}N_3O_2S·0.5C_2H_3N$	$Z = 16$
$M_r = 488.70$	$F_{000} = 4216$
Tetragonal, $I4_1/a$	$D_x = 1.117$ Mg m^{-3}
Hall symbol: -I 4ad	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 21.9895$ (17) Å	Cell parameters from 6978 reflections
$b = 21.9895$ (17) Å	$\theta = 2.2–22.8°$
$c = 24.035$ (3) Å	$\mu = 0.14$ mm^{-1}
$\alpha = 90°$	$T = 293$ (2) K
$\beta = 90°$	Block, yellow
$\gamma = 90°$	0.30 × 0.28 × 0.20 mm
$V = 11622.0$ (18) Å^3	

Data collection

Bruker SMART 1K CCD area-detector diffractometer	5766 independent reflections
Radiation source: fine-focus sealed tube	3108 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.063$
Detector resolution: 10 pixels mm^{-1}	$\theta_{max} = 26.1°$
$T = 293(2)$ K	$\theta_{min} = 1.9°$
φ and ω scans	$h = -17\rightarrow27$
Absorption correction: multi-scan (SADABS; Sheldrick, 2002)	$k = -27\rightarrow26$
$T_{min} = 0.769$, $T_{max} = 1.000$	$l = -29\rightarrow29$
31641 measured reflections	

Refinement

Refinement on F^2	H-atom parameters constrained

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.062$

$wR(F^2) = 0.216$

$S = 1.04$

5766 reflections

313 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

$w = 1/[\sigma^2(F_o^2) + (0.1113P)^2 + 3.0566P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.28$ e Å^{-3}

$\Delta\rho_{min} = -0.33$ e Å^{-3}

Extinction correction: none

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 $F^2 > 2$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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.12749 (4)	0.60119 (4)	0.03742 (3)	0.0730 (3)
O1	0.14047 (12)	0.57455 (12)	−0.01578 (8)	0.0999 (8)
O2	0.09863 (11)	0.65909 (10)	0.03769 (10)	0.0917 (7)
C1	−0.07243 (18)	0.68154 (17)	−0.01539 (14)	0.0931 (11)
H1	−0.0586	0.7005	0.0168	0.112*
N2	−0.03673 (11)	0.60214 (11)	0.07332 (10)	0.0693 (7)
N3	0.08473 (11)	0.55429 (11)	0.06978 (9)	0.0688 (6)
H3A	0.0798	0.5186	0.0559	0.083*
N4	0.0000	0.7500	0.2299 (5)	0.265 (6)
N1	−0.09302 (12)	0.59030 (12)	−0.06422 (11)	0.0794 (7)
C4	−0.11168 (15)	0.62558 (18)	−0.10696 (13)	0.0843 (9)
H4	−0.1257	0.6064	−0.1390	0.101*
C3	−0.11121 (16)	0.68721 (18)	−0.10611 (15)	0.0890 (10)
H3B	−0.1242	0.7093	−0.1369	0.107*
C2	−0.09163 (19)	0.71601 (18)	−0.05998 (16)	0.1019 (12)
H2	−0.0911	0.7583	−0.0582	0.122*
C5	−0.07375 (13)	0.61963 (14)	−0.01864 (12)	0.0687 (8)
C6	−0.05335 (13)	0.58042 (15)	0.02798 (12)	0.0715 (8)
H6A	−0.0530	0.5385	0.0232	0.086*
C7	−0.01480 (13)	0.56002 (14)	0.11595 (11)	0.0676 (8)

H7A	−0.0233	0.5181	0.1046	0.081*
C8	−0.04702 (16)	0.57368 (19)	0.17042 (14)	0.0940 (11)
H8A	−0.0418	0.6163	0.1795	0.113*
H8B	−0.0902	0.5660	0.1661	0.113*
C9	−0.02260 (19)	0.5352 (2)	0.21751 (14)	0.1026 (12)
H9A	−0.0432	0.5458	0.2518	0.123*
H9B	−0.0304	0.4926	0.2098	0.123*
C10	0.0446 (2)	0.5451 (2)	0.22403 (13)	0.1036 (12)
H10A	0.0600	0.5187	0.2531	0.124*
H10B	0.0520	0.5869	0.2353	0.124*
C11	0.07834 (16)	0.53241 (18)	0.17040 (13)	0.0898 (10)
H11A	0.0752	0.4894	0.1618	0.108*
H11B	0.1210	0.5420	0.1754	0.108*
C12	0.05348 (13)	0.56906 (13)	0.12206 (11)	0.0633 (7)
H12A	0.0607	0.6122	0.1300	0.076*
C13	0.19802 (13)	0.60672 (14)	0.07480 (11)	0.0660 (7)
C14	0.24248 (16)	0.56126 (15)	0.06689 (13)	0.0758 (8)
C15	0.23114 (18)	0.50094 (16)	0.03670 (16)	0.0942 (11)
H15A	0.1873	0.4977	0.0298	0.113*
C16	0.2634 (3)	0.5001 (2)	−0.0199 (2)	0.160 (2)
H16A	0.2503	0.5343	−0.0416	0.240*
H16B	0.2536	0.4632	−0.0392	0.240*
H16C	0.3066	0.5023	−0.0144	0.240*
C17	0.2495 (2)	0.44733 (19)	0.0724 (3)	0.145 (2)
H17A	0.2279	0.4488	0.1070	0.217*
H17B	0.2925	0.4490	0.0794	0.217*
H17C	0.2399	0.4102	0.0533	0.217*
C18	0.29944 (17)	0.57050 (17)	0.08867 (15)	0.0882 (10)
H18A	0.3291	0.5413	0.0819	0.106*
C19	0.31504 (17)	0.62005 (19)	0.11959 (16)	0.0926 (10)
C20	0.3802 (2)	0.6297 (3)	0.1408 (3)	0.1416 (18)
H20A	0.3949	0.5879	0.1455	0.170*
C21	0.3848 (3)	0.6544 (3)	0.1970 (2)	0.174 (2)
H21A	0.4269	0.6584	0.2070	0.261*
H21B	0.3649	0.6276	0.2227	0.261*
H21C	0.3656	0.6937	0.1982	0.261*
C22	0.4194 (3)	0.6531 (5)	0.0965 (3)	0.241 (5)
H22A	0.4599	0.6586	0.1106	0.362*
H22B	0.4040	0.6914	0.0836	0.362*
H22C	0.4202	0.6247	0.0661	0.362*
C23	0.27044 (17)	0.66180 (17)	0.13025 (14)	0.0859 (10)
H23A	0.2799	0.6951	0.1525	0.103*
C24	0.21147 (15)	0.65686 (14)	0.10948 (12)	0.0742 (8)
C25	0.16786 (18)	0.70501 (17)	0.13004 (16)	0.0975 (11)
H25A	0.1272	0.6927	0.1178	0.117*
C26	0.1808 (2)	0.7662 (2)	0.1032 (2)	0.1426 (18)
H26A	0.1788	0.7623	0.0634	0.214*
H26B	0.2206	0.7798	0.1138	0.214*
H26C	0.1511	0.7953	0.1154	0.214*

C27	0.1664 (3)	0.7066 (3)	0.1933 (2)	0.168 (2)
H27A	0.1567	0.6668	0.2073	0.252*
H27B	0.1361	0.7350	0.2055	0.252*
H27C	0.2055	0.7188	0.2071	0.252*
C28	0.0000	0.7500	0.1224 (3)	0.1063 (17)
C29	0.0000	0.7500	0.1818 (6)	0.153 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0865 (6)	0.0789 (5)	0.0537 (4)	0.0073 (4)	0.0018 (4)	0.0124 (4)
O1	0.133 (2)	0.1216 (19)	0.0456 (12)	0.0107 (16)	0.0040 (12)	0.0053 (11)
O2	0.1019 (16)	0.0725 (14)	0.1008 (17)	0.0140 (12)	−0.0035 (13)	0.0284 (12)
C1	0.123 (3)	0.082 (2)	0.074 (2)	0.002 (2)	−0.019 (2)	0.0050 (18)
N2	0.0696 (15)	0.0797 (16)	0.0586 (14)	−0.0029 (12)	−0.0122 (11)	0.0093 (12)
N3	0.0828 (16)	0.0666 (14)	0.0572 (13)	−0.0009 (12)	0.0009 (12)	0.0025 (11)
N4	0.251 (12)	0.356 (16)	0.188 (10)	−0.023 (10)	0.000	0.000
N1	0.0896 (18)	0.0865 (17)	0.0620 (15)	0.0000 (14)	−0.0183 (13)	0.0053 (13)
C4	0.092 (2)	0.103 (3)	0.0588 (19)	0.0096 (19)	−0.0131 (16)	0.0068 (17)
C3	0.094 (2)	0.100 (3)	0.073 (2)	0.016 (2)	−0.0032 (19)	0.026 (2)
C2	0.137 (3)	0.087 (2)	0.082 (2)	0.011 (2)	−0.022 (2)	0.010 (2)
C5	0.0682 (18)	0.079 (2)	0.0588 (17)	0.0029 (15)	−0.0073 (14)	0.0069 (14)
C6	0.0725 (19)	0.0752 (19)	0.0668 (19)	−0.0061 (15)	−0.0134 (15)	0.0092 (15)
C7	0.0730 (18)	0.0712 (18)	0.0586 (16)	−0.0110 (15)	−0.0134 (14)	0.0113 (14)
C8	0.083 (2)	0.122 (3)	0.077 (2)	−0.001 (2)	0.0104 (18)	0.026 (2)
C9	0.119 (3)	0.124 (3)	0.064 (2)	0.000 (2)	0.014 (2)	0.025 (2)
C10	0.129 (3)	0.132 (3)	0.0504 (18)	0.004 (3)	−0.0170 (19)	0.0176 (19)
C11	0.090 (2)	0.117 (3)	0.0625 (19)	0.016 (2)	−0.0151 (17)	0.0133 (18)
C12	0.0727 (18)	0.0670 (17)	0.0501 (15)	−0.0021 (14)	−0.0073 (13)	0.0026 (13)
C13	0.0754 (18)	0.0720 (18)	0.0506 (15)	0.0039 (15)	0.0152 (13)	0.0044 (13)
C14	0.082 (2)	0.077 (2)	0.0688 (18)	0.0065 (17)	0.0151 (16)	0.0061 (15)
C15	0.097 (2)	0.077 (2)	0.108 (3)	0.0118 (19)	0.024 (2)	−0.012 (2)
C16	0.190 (5)	0.142 (4)	0.147 (4)	−0.025 (4)	0.085 (4)	−0.058 (3)
C17	0.125 (4)	0.076 (3)	0.233 (6)	0.007 (2)	−0.018 (4)	0.014 (3)
C18	0.078 (2)	0.095 (3)	0.091 (2)	0.0136 (19)	0.0080 (19)	0.003 (2)
C19	0.083 (2)	0.105 (3)	0.090 (2)	−0.001 (2)	−0.0008 (19)	0.006 (2)
C20	0.101 (3)	0.174 (5)	0.149 (5)	−0.005 (3)	−0.021 (3)	−0.026 (4)
C21	0.163 (5)	0.246 (7)	0.114 (4)	−0.020 (5)	−0.046 (4)	0.013 (5)
C22	0.096 (4)	0.447 (14)	0.181 (7)	−0.063 (6)	0.010 (4)	−0.069 (8)
C23	0.089 (2)	0.094 (2)	0.075 (2)	−0.009 (2)	0.0057 (18)	−0.0062 (18)
C24	0.082 (2)	0.078 (2)	0.0624 (18)	0.0012 (16)	0.0182 (16)	0.0027 (15)
C25	0.092 (2)	0.095 (3)	0.105 (3)	0.000 (2)	0.023 (2)	−0.026 (2)
C26	0.129 (4)	0.089 (3)	0.210 (5)	0.017 (3)	0.030 (4)	−0.009 (3)
C27	0.181 (5)	0.198 (5)	0.125 (4)	0.016 (4)	0.055 (4)	−0.066 (4)
C28	0.115 (4)	0.099 (4)	0.105 (4)	0.019 (3)	0.000	0.000
C29	0.139 (7)	0.137 (6)	0.184 (10)	−0.001 (5)	0.000	0.000

Geometric parameters (Å, °)

S1—O2	1.423 (2)	C13—C24	1.414 (4)
S1—O1	1.435 (2)	C14—C18	1.373 (5)
S1—N3	1.598 (2)	C14—C15	1.532 (5)
S1—C13	1.796 (3)	C15—C17	1.512 (6)
C1—C5	1.364 (5)	C15—C16	1.536 (5)
C1—C2	1.379 (5)	C15—H15A	0.9800
C1—H1	0.9300	C16—H16A	0.9600
N2—C6	1.245 (4)	C16—H16B	0.9600
N2—C7	1.463 (3)	C16—H16C	0.9600
N3—C12	1.469 (3)	C17—H17A	0.9600
N3—H3A	0.8600	C17—H17B	0.9600
N4—C29	1.157 (12)	C17—H17C	0.9600
N1—C5	1.340 (4)	C18—C19	1.363 (5)
N1—C4	1.351 (4)	C18—H18A	0.9300
C4—C3	1.356 (5)	C19—C23	1.367 (5)
C4—H4	0.9300	C19—C20	1.535 (6)
C3—C2	1.347 (5)	C20—C21	1.460 (7)
C3—H3B	0.9300	C20—C22	1.465 (8)
C2—H2	0.9300	C20—H20A	0.9800
C5—C6	1.483 (4)	C21—H21A	0.9600
C6—H6A	0.9300	C21—H21B	0.9600
C7—C8	1.518 (4)	C21—H21C	0.9600
C7—C12	1.522 (4)	C22—H22A	0.9600
C7—H7A	0.9800	C22—H22B	0.9600
C8—C9	1.512 (5)	C22—H22C	0.9600
C8—H8A	0.9700	C23—C24	1.394 (5)
C8—H8B	0.9700	C23—H23A	0.9300
C9—C10	1.503 (5)	C24—C25	1.512 (5)
C9—H9A	0.9700	C25—C26	1.520 (6)
C9—H9B	0.9700	C25—C27	1.522 (6)
C10—C11	1.513 (5)	C25—H25A	0.9800
C10—H10A	0.9700	C26—H26A	0.9600
C10—H10B	0.9700	C26—H26B	0.9600
C11—C12	1.516 (4)	C26—H26C	0.9600
C11—H11A	0.9700	C27—H27A	0.9600
C11—H11B	0.9700	C27—H27B	0.9600
C12—H12A	0.9800	C27—H27C	0.9600
C13—C14	1.411 (4)	C28—C29	1.427 (13)
O2—S1—O1	117.26 (14)	C18—C14—C15	117.2 (3)
O2—S1—N3	108.23 (14)	C13—C14—C15	124.4 (3)
O1—S1—N3	106.69 (14)	C17—C15—C14	111.3 (4)
O2—S1—C13	108.81 (15)	C17—C15—C16	111.7 (4)
O1—S1—C13	107.55 (14)	C14—C15—C16	110.8 (3)
N3—S1—C13	107.96 (13)	C17—C15—H15A	107.6
C5—C1—C2	119.8 (3)	C14—C15—H15A	107.6
C5—C1—H1	120.1	C16—C15—H15A	107.6

C2—C1—H1	120.1	C15—C16—H16A	109.5
C6—N2—C7	117.8 (3)	C15—C16—H16B	109.5
C12—N3—S1	123.3 (2)	H16A—C16—H16B	109.5
C12—N3—H3A	118.3	C15—C16—H16C	109.5
S1—N3—H3A	118.3	H16A—C16—H16C	109.5
C5—N1—C4	116.2 (3)	H16B—C16—H16C	109.5
N1—C4—C3	124.1 (3)	C15—C17—H17A	109.5
N1—C4—H4	118.0	C15—C17—H17B	109.5
C3—C4—H4	118.0	H17A—C17—H17B	109.5
C2—C3—C4	119.0 (3)	C15—C17—H17C	109.5
C2—C3—H3B	120.5	H17A—C17—H17C	109.5
C4—C3—H3B	120.5	H17B—C17—H17C	109.5
C3—C2—C1	118.6 (4)	C19—C18—C14	123.8 (3)
C3—C2—H2	120.7	C19—C18—H18A	118.1
C1—C2—H2	120.7	C14—C18—H18A	118.1
N1—C5—C1	122.3 (3)	C18—C19—C23	117.3 (3)
N1—C5—C6	115.7 (3)	C18—C19—C20	121.7 (4)
C1—C5—C6	122.0 (3)	C23—C19—C20	121.0 (4)
N2—C6—C5	121.8 (3)	C21—C20—C22	120.0 (5)
N2—C6—H6A	119.1	C21—C20—C19	115.1 (5)
C5—C6—H6A	119.1	C22—C20—C19	110.9 (5)
N2—C7—C8	109.0 (3)	C21—C20—H20A	102.6
N2—C7—C12	108.1 (2)	C22—C20—H20A	102.6
C8—C7—C12	110.6 (2)	C19—C20—H20A	102.6
N2—C7—H7A	109.7	C20—C21—H21A	109.5
C8—C7—H7A	109.7	C20—C21—H21B	109.5
C12—C7—H7A	109.7	H21A—C21—H21B	109.5
C9—C8—C7	111.6 (3)	C20—C21—H21C	109.5
C9—C8—H8A	109.3	H21A—C21—H21C	109.5
C7—C8—H8A	109.3	H21B—C21—H21C	109.5
C9—C8—H8B	109.3	C20—C22—H22A	109.5
C7—C8—H8B	109.3	C20—C22—H22B	109.5
H8A—C8—H8B	108.0	H22A—C22—H22B	109.5
C10—C9—C8	110.2 (3)	C20—C22—H22C	109.5
C10—C9—H9A	109.6	H22A—C22—H22C	109.5
C8—C9—H9A	109.6	H22B—C22—H22C	109.5
C10—C9—H9B	109.6	C19—C23—C24	123.2 (3)
C8—C9—H9B	109.6	C19—C23—H23A	118.4
H9A—C9—H9B	108.1	C24—C23—H23A	118.4
C9—C10—C11	111.5 (3)	C23—C24—C13	117.8 (3)
C9—C10—H10A	109.3	C23—C24—C25	114.7 (3)
C11—C10—H10A	109.3	C13—C24—C25	127.3 (3)
C9—C10—H10B	109.3	C24—C25—C26	111.3 (3)
C11—C10—H10B	109.3	C24—C25—C27	110.8 (4)
H10A—C10—H10B	108.0	C26—C25—C27	114.1 (4)
C10—C11—C12	112.2 (3)	C24—C25—H25A	106.7
C10—C11—H11A	109.2	C26—C25—H25A	106.7
C12—C11—H11A	109.2	C27—C25—H25A	106.7
C10—C11—H11B	109.2	C25—C26—H26A	109.5

C12—C11—H11B	109.2	C25—C26—H26B	109.5
H11A—C11—H11B	107.9	H26A—C26—H26B	109.5
N3—C12—C11	111.7 (2)	C25—C26—H26C	109.5
N3—C12—C7	110.5 (2)	H26A—C26—H26C	109.5
C11—C12—C7	111.1 (2)	H26B—C26—H26C	109.5
N3—C12—H12A	107.8	C25—C27—H27A	109.5
C11—C12—H12A	107.8	C25—C27—H27B	109.5
C7—C12—H12A	107.8	H27A—C27—H27B	109.5
C14—C13—C24	119.1 (3)	C25—C27—H27C	109.5
C14—C13—S1	118.9 (2)	H27A—C27—H27C	109.5
C24—C13—S1	121.9 (2)	H27B—C27—H27C	109.5
C18—C14—C13	118.4 (3)	N4—C29—C28	180.000 (3)
O2—S1—N3—C12	−42.8 (3)	O2—S1—C13—C24	14.6 (3)
O1—S1—N3—C12	−169.8 (2)	O1—S1—C13—C24	142.6 (2)
C13—S1—N3—C12	74.8 (2)	N3—S1—C13—C24	−102.6 (2)
C5—N1—C4—C3	0.7 (5)	C24—C13—C14—C18	−6.5 (4)
N1—C4—C3—C2	−0.7 (6)	S1—C13—C14—C18	170.1 (2)
C4—C3—C2—C1	0.4 (6)	C24—C13—C14—C15	171.8 (3)
C5—C1—C2—C3	−0.2 (6)	S1—C13—C14—C15	−11.6 (4)
C4—N1—C5—C1	−0.5 (5)	C18—C14—C15—C17	52.0 (4)
C4—N1—C5—C6	−180.0 (3)	C13—C14—C15—C17	−126.4 (4)
C2—C1—C5—N1	0.3 (6)	C18—C14—C15—C16	−72.9 (5)
C2—C1—C5—C6	179.7 (3)	C13—C14—C15—C16	108.7 (4)
C7—N2—C6—C5	−177.3 (3)	C13—C14—C18—C19	2.8 (5)
N1—C5—C6—N2	−177.1 (3)	C15—C14—C18—C19	−175.6 (3)
C1—C5—C6—N2	3.5 (5)	C14—C18—C19—C23	1.6 (6)
C6—N2—C7—C8	−130.4 (3)	C14—C18—C19—C20	−177.2 (4)
C6—N2—C7—C12	109.4 (3)	C18—C19—C20—C21	−140.9 (5)
N2—C7—C8—C9	−175.2 (3)	C23—C19—C20—C21	40.4 (7)
C12—C7—C8—C9	−56.6 (4)	C18—C19—C20—C22	78.8 (7)
C7—C8—C9—C10	57.6 (4)	C23—C19—C20—C22	−100.0 (6)
C8—C9—C10—C11	−56.1 (5)	C18—C19—C23—C24	−2.4 (5)
C9—C10—C11—C12	54.9 (5)	C20—C19—C23—C24	176.5 (4)
S1—N3—C12—C11	−112.8 (3)	C19—C23—C24—C13	−1.4 (5)
S1—N3—C12—C7	122.9 (2)	C19—C23—C24—C25	175.2 (3)
C10—C11—C12—N3	−177.4 (3)	C14—C13—C24—C23	5.8 (4)
C10—C11—C12—C7	−53.5 (4)	S1—C13—C24—C23	−170.7 (2)
N2—C7—C12—N3	−62.3 (3)	C14—C13—C24—C25	−170.3 (3)
C8—C7—C12—N3	178.5 (3)	S1—C13—C24—C25	13.2 (4)
N2—C7—C12—C11	173.1 (2)	C23—C24—C25—C26	73.3 (4)
C8—C7—C12—C11	54.0 (3)	C13—C24—C25—C26	−110.5 (4)
O2—S1—C13—C14	−161.9 (2)	C23—C24—C25—C27	−54.8 (5)
O1—S1—C13—C14	−34.0 (3)	C13—C24—C25—C27	121.4 (4)
N3—S1—C13—C14	80.8 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3A···N1^{i}	0.86	2.42	3.188 (4)	149

Symmetry codes: (i) −*x*, −*y*+1, −*z*.

Fig. 1

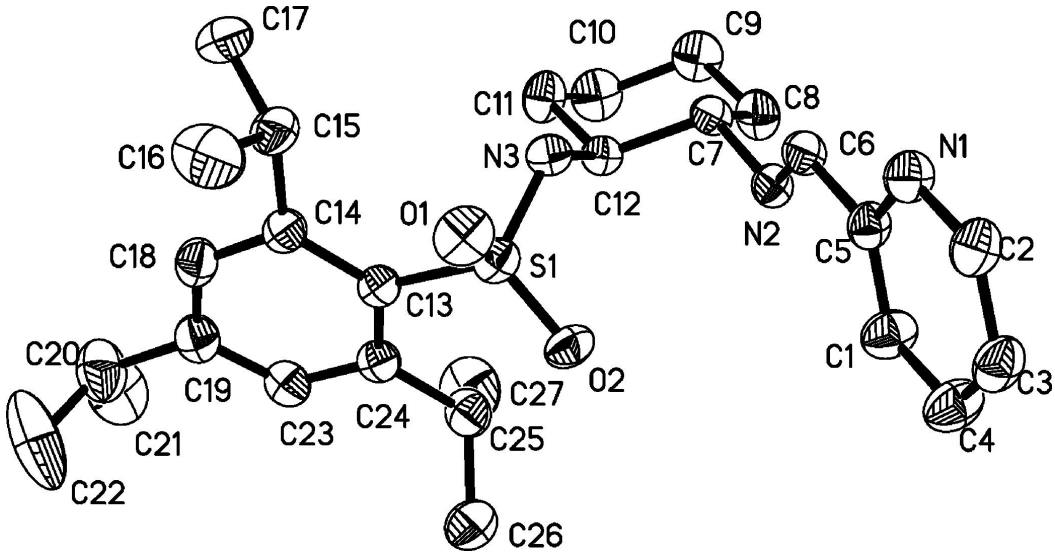

Fig. 2