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4-{(4*Z*)-4-[(2*Z*)-3-(4-Fluoroanilino)-1-hydroxybut-2-en-1-ylidene]-3-methyl-5-oxo-4,5-dihydro-1*H*-pyrazol-1-yl}-benzenesulfonamide

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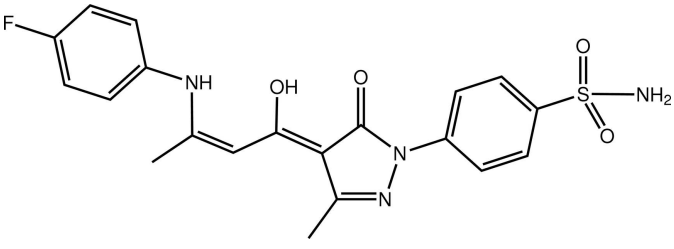
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; R factor = 0.059; wR factor = 0.146; data-to-parameter ratio = 14.8.

In the title compound, $C_{20}H_{19}FN_4O_4S$, the pyrazole and benzenesulfonamide rings are coplanar [dihedral angle = 5.02 (15)°] but this planarity does not extend over the entire molecule, the dihedral angle between the terminal six-membered rings being 33.24 (14)°. Intramolecular hydroxy–hydroxy O—H···O and amine–hydroxy N—H···O hydrogen bonds, as a well as a tight C—H···O(carbonyl) interaction, lead to a sequence of three fused S(6) rings. Supramolecular chains along the a axis feature in the crystal packing; these chains are stabilized by amine–sulfonamide N—H···O and amine–pyrazole N—H···N hydrogen bonds.

Related literature

For background to the synthesis, see: Gelin *et al.* (1983); Bendaas *et al.* (1999). For related structures, see: Asiri, Al-Youbi, Alamry *et al.* (2011); Asiri, Al-Youbi, Faidallah *et al.* (2011).



Experimental

Crystal data

$C_{20}H_{19}FN_4O_4S$
M_r = 430.45
Triclinic, $P\overline{1}$
a = 7.8121 (5) Å
b = 10.0137 (8) Å
c = 12.6003 (9) Å
α = 97.950 (6)°
β = 104.632 (6)°
γ = 98.394 (6)°
V = 927.58 (12) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 100 K
0.25 × 0.10 × 0.02 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.946, T_{max} = 0.996
6559 measured reflections
4240 independent reflections
2935 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.146
S = 1.01
4240 reflections
287 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H1···O1	0.85 (1)	1.71 (2)	2.522 (3)	161 (4)
N3—H3···O2	0.88 (1)	1.95 (2)	2.662 (3)	137 (3)
C2—H2···O1	0.95	2.26	2.917 (4)	126
N4—H41···N2^{i}	0.88 (1)	2.14 (1)	2.999 (3)	167 (3)
N4—H42···O3^{ii}	0.88 (1)	2.08 (1)	2.943 (3)	169 (3)

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

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; 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: HG5177).

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supplementary materials

Acta Cryst. (2012). E**68**, o762–o763 [doi:10.1107/S1600536812006502]

4-{(4*Z*)-4-[(2*Z*)-3-(4-Fluoroanilino)-1-hydroxybut-2-en-1-ylidene]-3-methyl-5-oxo-4,5-dihydro-1*H*-pyrazol-1-yl}benzenesulfonamide

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Comment

In connection with a recent structural studies (Asiri, Al-Youbi, Alamry *et al.*, 2011; Asiri, Al-Youbi, Faidallah *et al.*, 2011), the title compound, 4-{4-[3-(4-fluoroanilino)-1-hydroxybut-2-enylidene]-3-methyl-5-oxo-4,5-dihydro-1*H*-pyrazol-1-yl}benzenesulfonamide (I), was prepared as a part of on-going investigations of reactions between pyrazoles and aniline derivatives based on literature procedures (Gelin *et al.*, 1983; Bendaas *et al.*, 1999).

In (I), Fig. 1, the pyrazolyl and benzenesulfonamide rings are co-planar as seen in dihedral angle of 5.02 (15)°. The planarity extends to the rest of the molecule with the exception of the terminal benzene ring; the dihedral angle between the terminal six-membered rings being 33.24 (14)°. The observed planarity is accounted for by the presence of intramolecular O—H···O and N—H···O hydrogen bonds involving the central hydroxyl-O2 atom functioning as both an acceptor and as a donor, Table 1. These interactions are complemented by a tight C—H···O1 interaction, Table 1. The intramolecular interactions lead to a sequence of three fused *S*(6) rings.

The molecules are connected into a supramolecular chain along the *a* axis in the crystal packing, Fig. 2 and Table 1. Both amide-H atoms form hydrogen bonds, one to a sulfonamide-O3 atom and the other to a pyrazolyl-N2 atom. Centrosymmetrically related molecules associate *via* an eight-membered $\{\cdots HNSO\}_2$ synthon. These are linked to translationally related molecules *via* N–H···N hydrogen bonds which lead to the formation of 22-membered $\{\cdots HNH\cdots OSC_4N_2\}_2$ synthons which encompass two of the aforementioned N—H···O hydrogen bonds.

Experimental

A solution of 4-acetoacetyl-5-hydroxy-3-methyl-1-*p*-sulfamylphenypyrazole (1.7 g, 0.005 mol) and 4-fluoroaniline (0.55 g, 0.005 mol) in ethanol (25 ml) was refluxed for 2 h. The precipitate, obtained from the hot solution, was collected, washed with methanol and recrystallized from ethanol-benzene to yield yellow crystals; *M*.pt: 411–412 K.

Refinement

Carbon-bound H-atoms were placed in calculated positions [C—H = 0.95 to 0.98 Å, U_{iso}(H) = 1.2 to 1.5U_{eq}(C)] and were included in the refinement in the riding model approximation. The N—H and O—H-atoms were located in a difference Fourier map, and were refined with distance restraints of N—H = 0.88±0.01 and O—H = 0.84±0.01 Å, respectively; their U_{iso} values were refined.

Computing details

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO* (Agilent, 2011); data reduction: *CrysAlis PRO* (Agilent, 2011); 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).

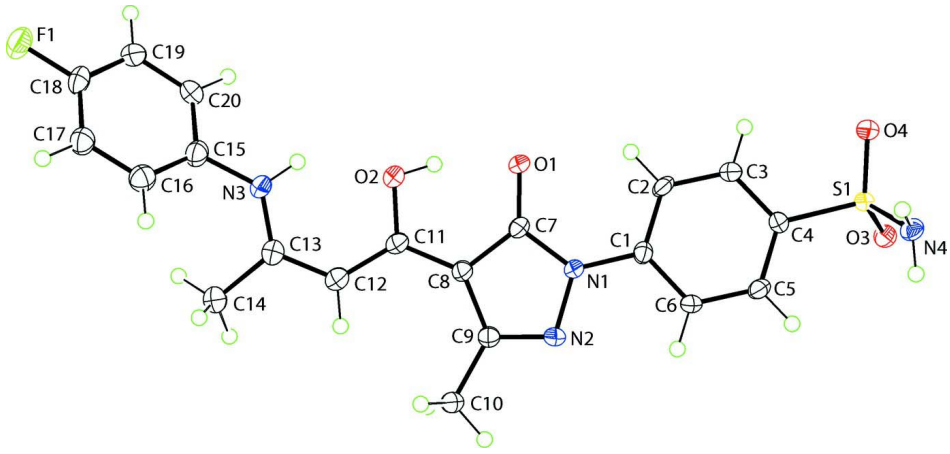

Figure 1

The molecular structure of (I) showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level.

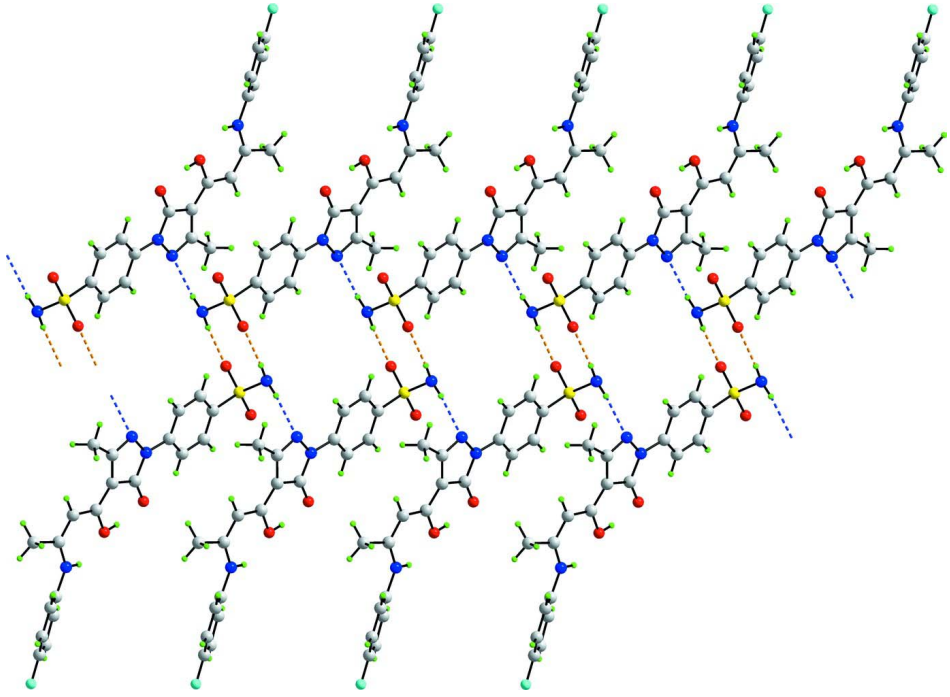

Figure 2

A view of a supramolecular chain along the *a* axis in (I) mediated by N—H···O and N—H···N hydrogen bonds shown as orange and blue dashed lines, respectively.

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Crystal data

$C_{20}H_{19}FN_4O_4S$
$M_r = 430.45$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.8121$ (5) Å
$b = 10.0137$ (8) Å
$c = 12.6003$ (9) Å
$\alpha = 97.950$ (6)°
$\beta = 104.632$ (6)°
$\gamma = 98.394$ (6)°
$V = 927.58$ (12) Å^3
$Z = 2$
$F(000) = 448$
$D_x = 1.541$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1846 reflections
$\theta = 2.4$–27.5°
$\mu = 0.22$ mm^{-1}
$T = 100$ K
Prism, yellow
0.25 × 0.10 × 0.02 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.4041 pixels mm^{-1}
ω scan
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
$T_{min} = 0.946$, $T_{max} = 0.996$
6559 measured reflections
4240 independent reflections
2935 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$
$\theta_{max} = 27.6$°, $\theta_{min} = 2.4$°
$h = -10 \rightarrow 7$
$k = -12 \rightarrow 13$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.059$
$wR(F^2) = 0.146$
$S = 1.01$
4240 reflections
287 parameters
4 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0548P)^2 + 0.375P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.47$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	1.14758 (9)	0.18251 (7)	0.13099 (5)	0.01909 (19)
F1	0.3342 (3)	0.78774 (18)	1.20106 (14)	0.0361 (5)
O1	0.7345 (3)	0.41000 (19)	0.53049 (16)	0.0245 (5)
O2	0.5322 (3)	0.4509 (2)	0.65439 (16)	0.0267 (5)
H1	0.608 (4)	0.457 (4)	0.617 (3)	0.057 (12)*
O3	1.0480 (3)	0.17118 (19)	0.01577 (15)	0.0218 (5)
O4	1.2886 (3)	0.2998 (2)	0.18161 (16)	0.0262 (5)
N1	0.6195 (3)	0.2035 (2)	0.39856 (18)	0.0181 (5)
N2	0.4693 (3)	0.0958 (2)	0.37289 (18)	0.0194 (5)
N3	0.3372 (3)	0.4895 (2)	0.7974 (2)	0.0246 (6)

H3	0.429 (3)	0.519 (3)	0.772 (2)	0.026 (9)*
N4	1.2349 (3)	0.0473 (2)	0.13729 (19)	0.0214 (5)
H41	1.299 (3)	0.047 (3)	0.2055 (13)	0.026*
H42	1.156 (3)	−0.025 (2)	0.098 (2)	0.026*
C1	0.7495 (4)	0.1957 (3)	0.3386 (2)	0.0184 (6)
C2	0.8925 (4)	0.3055 (3)	0.3569 (2)	0.0207 (6)
H2	0.9062	0.3844	0.4119	0.025*
C3	1.0138 (4)	0.2982 (3)	0.2943 (2)	0.0208 (6)
H3A	1.1116	0.3725	0.3067	0.025*
C4	0.9944 (4)	0.1833 (3)	0.2133 (2)	0.0183 (6)
C5	0.8533 (4)	0.0721 (3)	0.1959 (2)	0.0198 (6)
H5	0.8402	−0.0066	0.1409	0.024*
C6	0.7327 (4)	0.0778 (3)	0.2596 (2)	0.0185 (6)
H6	0.6385	0.0016	0.2498	0.022*
C7	0.6167 (4)	0.3021 (3)	0.4854 (2)	0.0190 (6)
C8	0.4559 (4)	0.2561 (3)	0.5145 (2)	0.0191 (6)
C9	0.3752 (4)	0.1281 (3)	0.4419 (2)	0.0194 (6)
C10	0.2070 (4)	0.0316 (3)	0.4376 (2)	0.0224 (6)
H10A	0.1031	0.0764	0.4172	0.034*
H10B	0.2166	0.0062	0.5110	0.034*
H10C	0.1914	−0.0512	0.3819	0.034*
C11	0.4130 (4)	0.3362 (3)	0.6027 (2)	0.0215 (6)
C12	0.2592 (4)	0.3066 (3)	0.6396 (2)	0.0252 (7)
H12	0.1707	0.2292	0.5978	0.030*
C13	0.2232 (4)	0.3787 (3)	0.7311 (2)	0.0233 (6)
C14	0.0456 (4)	0.3322 (3)	0.7541 (3)	0.0316 (8)
H14A	−0.0467	0.2940	0.6834	0.047*
H14B	0.0101	0.4107	0.7929	0.047*
H14C	0.0581	0.2617	0.8008	0.047*
C15	0.3261 (4)	0.5620 (3)	0.9014 (2)	0.0273 (7)
C16	0.2655 (4)	0.4976 (3)	0.9798 (3)	0.0288 (7)
H16	0.2238	0.4011	0.9648	0.035*
C17	0.2665 (4)	0.5744 (3)	1.0786 (2)	0.0281 (7)
H17	0.2213	0.5319	1.1315	0.034*
C18	0.3323 (4)	0.7119 (3)	1.1012 (2)	0.0252 (7)
C19	0.3989 (4)	0.7777 (3)	1.0272 (2)	0.0280 (7)
H19	0.4477	0.8733	1.0453	0.034*
C20	0.3932 (4)	0.7016 (3)	0.9259 (2)	0.0257 (7)
H20	0.4356	0.7454	0.8727	0.031*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0177 (4)	0.0186 (4)	0.0193 (4)	−0.0007 (3)	0.0069 (3)	−0.0013 (3)
F1	0.0487 (12)	0.0327 (10)	0.0289 (10)	0.0100 (9)	0.0165 (9)	−0.0006 (8)
O1	0.0214 (11)	0.0215 (10)	0.0259 (11)	−0.0032 (9)	0.0089 (9)	−0.0082 (8)
O2	0.0252 (12)	0.0268 (11)	0.0250 (11)	−0.0012 (10)	0.0107 (9)	−0.0059 (9)
O3	0.0224 (10)	0.0235 (11)	0.0189 (10)	0.0035 (9)	0.0055 (8)	0.0029 (8)
O4	0.0244 (11)	0.0233 (11)	0.0281 (11)	−0.0044 (9)	0.0119 (9)	−0.0040 (8)
N1	0.0169 (12)	0.0174 (12)	0.0177 (12)	0.0004 (10)	0.0053 (9)	−0.0020 (9)

N2	0.0171 (12)	0.0186 (12)	0.0197 (12)	−0.0013 (10)	0.0044 (10)	0.0000 (9)
N3	0.0236 (14)	0.0240 (13)	0.0243 (13)	0.0026 (11)	0.0092 (11)	−0.0042 (10)
N4	0.0205 (13)	0.0233 (13)	0.0170 (12)	0.0033 (11)	0.0022 (10)	−0.0009 (10)
C1	0.0181 (14)	0.0220 (14)	0.0156 (13)	0.0053 (12)	0.0053 (11)	0.0018 (11)
C2	0.0246 (15)	0.0169 (14)	0.0172 (14)	0.0033 (12)	0.0045 (12)	−0.0047 (10)
C3	0.0188 (14)	0.0181 (14)	0.0231 (15)	0.0003 (12)	0.0052 (12)	−0.0001 (11)
C4	0.0160 (14)	0.0200 (14)	0.0192 (14)	0.0029 (12)	0.0063 (11)	0.0023 (11)
C5	0.0208 (15)	0.0174 (14)	0.0182 (14)	0.0027 (12)	0.0030 (11)	−0.0018 (10)
C6	0.0164 (14)	0.0174 (14)	0.0185 (14)	−0.0013 (11)	0.0036 (11)	0.0000 (10)
C7	0.0213 (15)	0.0195 (14)	0.0146 (13)	0.0029 (12)	0.0042 (11)	−0.0002 (10)
C8	0.0177 (14)	0.0209 (14)	0.0175 (14)	0.0028 (12)	0.0044 (11)	0.0010 (11)
C9	0.0179 (14)	0.0203 (14)	0.0186 (14)	0.0023 (12)	0.0039 (11)	0.0019 (11)
C10	0.0239 (15)	0.0200 (14)	0.0214 (15)	−0.0005 (12)	0.0070 (12)	0.0012 (11)
C11	0.0226 (15)	0.0211 (14)	0.0176 (14)	0.0021 (12)	0.0036 (12)	−0.0008 (11)
C12	0.0251 (16)	0.0254 (16)	0.0222 (15)	0.0021 (13)	0.0059 (12)	−0.0011 (12)
C13	0.0245 (15)	0.0252 (15)	0.0215 (15)	0.0072 (13)	0.0074 (12)	0.0041 (12)
C14	0.0278 (17)	0.0327 (18)	0.0347 (18)	0.0034 (15)	0.0146 (14)	−0.0008 (13)
C15	0.0244 (16)	0.0315 (17)	0.0254 (16)	0.0072 (14)	0.0083 (13)	−0.0006 (12)
C16	0.0314 (17)	0.0256 (16)	0.0308 (17)	0.0067 (14)	0.0105 (14)	0.0048 (13)
C17	0.0290 (17)	0.0287 (17)	0.0284 (17)	0.0074 (14)	0.0110 (14)	0.0037 (13)
C18	0.0260 (16)	0.0307 (16)	0.0207 (15)	0.0123 (14)	0.0077 (12)	0.0014 (12)
C19	0.0263 (16)	0.0247 (16)	0.0302 (17)	0.0003 (14)	0.0090 (13)	−0.0016 (12)
C20	0.0203 (15)	0.0287 (16)	0.0285 (16)	0.0021 (13)	0.0096 (13)	0.0039 (13)

Geometric parameters (Å, º)

S1—O4	1.4353 (19)	C6—H6	0.9500
S1—O3	1.4437 (19)	C7—C8	1.427 (4)
S1—N4	1.605 (3)	C8—C11	1.417 (4)
S1—C4	1.770 (3)	C8—C9	1.423 (4)
F1—C18	1.372 (3)	C9—C10	1.497 (4)
O1—C7	1.270 (3)	C10—H10A	0.9800
O2—C11	1.336 (3)	C10—H10B	0.9800
O2—H1	0.848 (10)	C10—H10C	0.9800
N1—C7	1.375 (3)	C11—C12	1.402 (4)
N1—N2	1.410 (3)	C12—C13	1.387 (4)
N1—C1	1.415 (3)	C12—H12	0.9500
N2—C9	1.311 (4)	C13—C14	1.508 (4)
N3—C13	1.342 (4)	C14—H14A	0.9800
N3—C15	1.436 (4)	C14—H14B	0.9800
N3—H3	0.881 (10)	C14—H14C	0.9800
N4—H41	0.878 (10)	C15—C20	1.382 (4)
N4—H42	0.875 (10)	C15—C16	1.393 (4)
C1—C2	1.397 (4)	C16—C17	1.368 (4)
C1—C6	1.401 (4)	C16—H16	0.9500
C2—C3	1.381 (4)	C17—C18	1.361 (4)
C2—H2	0.9500	C17—H17	0.9500
C3—C4	1.391 (4)	C18—C19	1.375 (4)
C3—H3A	0.9500	C19—C20	1.380 (4)
C4—C5	1.398 (4)	C19—H19	0.9500

C5—C6	1.386 (4)	C20—H20	0.9500
C5—H5	0.9500		

O4—S1—O3	118.53 (11)	N2—C9—C10	119.3 (2)
O4—S1—N4	108.00 (13)	C8—C9—C10	128.9 (3)
O3—S1—N4	106.03 (12)	C9—C10—H10A	109.5
O4—S1—C4	106.19 (12)	C9—C10—H10B	109.5
O3—S1—C4	108.51 (13)	H10A—C10—H10B	109.5
N4—S1—C4	109.38 (13)	C9—C10—H10C	109.5
C11—O2—H1	105 (3)	H10A—C10—H10C	109.5
C7—N1—N2	111.1 (2)	H10B—C10—H10C	109.5
C7—N1—C1	129.7 (2)	O2—C11—C12	117.8 (3)
N2—N1—C1	119.2 (2)	O2—C11—C8	115.8 (2)
C9—N2—N1	106.2 (2)	C12—C11—C8	126.4 (2)
C13—N3—C15	127.8 (2)	C13—C12—C11	126.6 (3)
C13—N3—H3	114 (2)	C13—C12—H12	116.7
C15—N3—H3	118 (2)	C11—C12—H12	116.7
S1—N4—H41	111 (2)	N3—C13—C12	122.7 (3)
S1—N4—H42	110 (2)	N3—C13—C14	119.2 (3)
H41—N4—H42	121 (3)	C12—C13—C14	118.1 (3)
C2—C1—C6	120.2 (2)	C13—C14—H14A	109.5
C2—C1—N1	120.2 (2)	C13—C14—H14B	109.5
C6—C1—N1	119.6 (2)	H14A—C14—H14B	109.5
C3—C2—C1	119.3 (3)	C13—C14—H14C	109.5
C3—C2—H2	120.3	H14A—C14—H14C	109.5
C1—C2—H2	120.3	H14B—C14—H14C	109.5
C2—C3—C4	120.7 (2)	C20—C15—C16	119.7 (3)
C2—C3—H3A	119.6	C20—C15—N3	116.5 (2)
C4—C3—H3A	119.6	C16—C15—N3	123.6 (3)
C3—C4—C5	120.2 (3)	C17—C16—C15	119.5 (3)
C3—C4—S1	118.9 (2)	C17—C16—H16	120.2
C5—C4—S1	120.9 (2)	C15—C16—H16	120.2
C6—C5—C4	119.4 (2)	C18—C17—C16	119.9 (3)
C6—C5—H5	120.3	C18—C17—H17	120.0
C4—C5—H5	120.3	C16—C17—H17	120.0
C5—C6—C1	120.1 (2)	C17—C18—F1	119.4 (2)
C5—C6—H6	120.0	C17—C18—C19	122.0 (3)
C1—C6—H6	120.0	F1—C18—C19	118.6 (3)
O1—C7—N1	126.8 (2)	C18—C19—C20	118.4 (3)
O1—C7—C8	127.7 (2)	C18—C19—H19	120.8
N1—C7—C8	105.5 (2)	C20—C19—H19	120.8
C11—C8—C9	134.9 (3)	C19—C20—C15	120.4 (3)
C11—C8—C7	119.6 (2)	C19—C20—H20	119.8
C9—C8—C7	105.5 (2)	C15—C20—H20	119.8
N2—C9—C8	111.8 (2)		

C7—N1—N2—C9	0.5 (3)	N1—C7—C8—C9	1.2 (3)
C1—N1—N2—C9	178.6 (2)	N1—N2—C9—C8	0.3 (3)
C7—N1—C1—C2	−7.0 (4)	N1—N2—C9—C10	−178.6 (2)

N2—N1—C1—C2	175.4 (2)	C11—C8—C9—N2	−179.4 (3)
C7—N1—C1—C6	173.8 (3)	C7—C8—C9—N2	−1.0 (3)
N2—N1—C1—C6	−3.8 (4)	C11—C8—C9—C10	−0.6 (6)
C6—C1—C2—C3	1.8 (4)	C7—C8—C9—C10	177.8 (3)
N1—C1—C2—C3	−177.4 (3)	C9—C8—C11—O2	177.0 (3)
C1—C2—C3—C4	0.3 (4)	C7—C8—C11—O2	−1.2 (4)
C2—C3—C4—C5	−1.4 (4)	C9—C8—C11—C12	−3.1 (6)
C2—C3—C4—S1	177.1 (2)	C7—C8—C11—C12	178.6 (3)
O4—S1—C4—C3	10.3 (3)	O2—C11—C12—C13	−5.5 (5)
O3—S1—C4—C3	−118.1 (2)	C8—C11—C12—C13	174.7 (3)
N4—S1—C4—C3	126.6 (2)	C15—N3—C13—C12	−171.6 (3)
O4—S1—C4—C5	−171.2 (2)	C15—N3—C13—C14	10.4 (5)
O3—S1—C4—C5	60.3 (3)	C11—C12—C13—N3	−0.2 (5)
N4—S1—C4—C5	−54.9 (3)	C11—C12—C13—C14	177.9 (3)
C3—C4—C5—C6	0.3 (4)	C13—N3—C15—C20	−148.1 (3)
S1—C4—C5—C6	−178.1 (2)	C13—N3—C15—C16	37.0 (5)
C4—C5—C6—C1	1.8 (4)	C20—C15—C16—C17	2.6 (5)
C2—C1—C6—C5	−2.9 (4)	N3—C15—C16—C17	177.3 (3)
N1—C1—C6—C5	176.3 (3)	C15—C16—C17—C18	−2.3 (5)
N2—N1—C7—O1	178.0 (3)	C16—C17—C18—F1	−179.4 (3)
C1—N1—C7—O1	0.2 (5)	C16—C17—C18—C19	0.0 (5)
N2—N1—C7—C8	−1.1 (3)	C17—C18—C19—C20	1.9 (5)
C1—N1—C7—C8	−178.9 (3)	F1—C18—C19—C20	−178.6 (3)
O1—C7—C8—C11	0.9 (5)	C18—C19—C20—C15	−1.6 (5)
N1—C7—C8—C11	179.9 (2)	C16—C15—C20—C19	−0.6 (5)
O1—C7—C8—C9	−177.8 (3)	N3—C15—C20—C19	−175.7 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H1···O1	0.85 (1)	1.71 (2)	2.522 (3)	161 (4)
N3—H3···O2	0.88 (1)	1.95 (2)	2.662 (3)	137 (3)
C2—H2···O1	0.95	2.26	2.917 (4)	126
N4—H41···N2^{i}	0.88 (1)	2.14 (1)	2.999 (3)	167 (3)
N4—H42···O3^{ii}	0.88 (1)	2.08 (1)	2.943 (3)	169 (3)

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