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ISSN 2414-3146

1,5-Dimethyl-3′,5′-diphenyl-1,5-dihydro-3′*H*-spiro-[pyrazolo[3,4-*d*]pyrimidine-4,2′-[1,3,4]-thiadiazole]

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Received 6 June 2017
Accepted 13 July 2017

Edited by W. T. A. Harrison, University of Aberdeen, Scotland

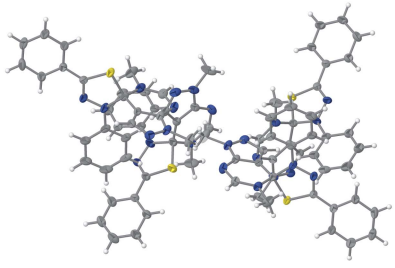
Keywords: crystal structure; hydrogen bond; pyrimidine; thiadiazole.

CCDC reference: 1562???

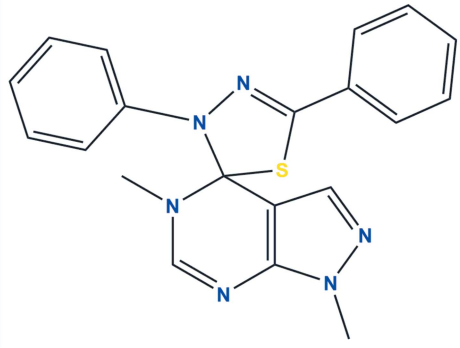
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title compound, $C_{20}H_{18}N_6S$, consists of four independent molecules with similar conformations [dihedral angles between the ring systems linked *via* the spiro-C atom = 87.14 (17), 87.09 (16), 88.41 (17) and 88.39 (17)°]. In the crystal, C—H···N hydrogen bonds bind the molecules into double chains running along the *a*-axis direction.

3D view



Chemical scheme



Structure description

As a continuation of our research into hydantoin derivatives (El Fal *et al.*, 2015, 2017), the title compound (Figs. 1 and 2) was prepared and its crystal structure is reported here.

The asymmetric unit consists of four independent molecules, *A*–*D* (containing atoms S1–S4, respectively), with similar conformations. The dihedral angles between the thiadiazole ring and the pyrazine–pyrimidine ring system linked by the spiro-C atoms are 87.14 (17) (molecule *A*), 87.09 (16) (*B*), 88.41 (17) (*C*) and 88.39 (17)° (*D*). Further similarity is evidenced in terms of the dihedral angles between the thiadiazole ring and its pendant phenyl groups: 15.6 (2) and 12.0 (2) (molecule *A*), 16.6 (2) and 13.6 (2) (*B*), 12.6 (2) and 15.2 (2) (*C*), and 13.1 (2) and 17.0 (2)° (*D*). The conformations of the molecules containing atoms S1 and S3 may differ slightly from those with S2 and S4 in terms of the orientation of the methyl groups attached to the pyrimidine rings (Table 1), assuming that the locations of the H atoms are reliably determined in terms of the rotating-rigid-group refinement model. Puckering analyses of the five-membered rings containing sulfur gave parameters $Q(2) = 0.136$ (4) Å and $\varphi(2) = 329.2$ (16)° (envelope on atom C2) for the S1-containing ring, $Q(2) = 0.144$ (4) Å and $\varphi(2) = 143.0$ (15)° (envelope on C22) for the S2-containing ring, and 0.078 (4) Å and $\varphi(2) = 322$ (3)° (envelope on C42) for the S3-containing ring, while the S4-containing ring was too close to being planar for a meaningful puckering analysis.

Table 1
Selected torsion angles (°).

C4—N6—C7—H7*A*	−79	C24—N12—C27—H27*B*	−112
C44—N18—C47—H47*A*	109	C64—N24—C67—H67*B*	79

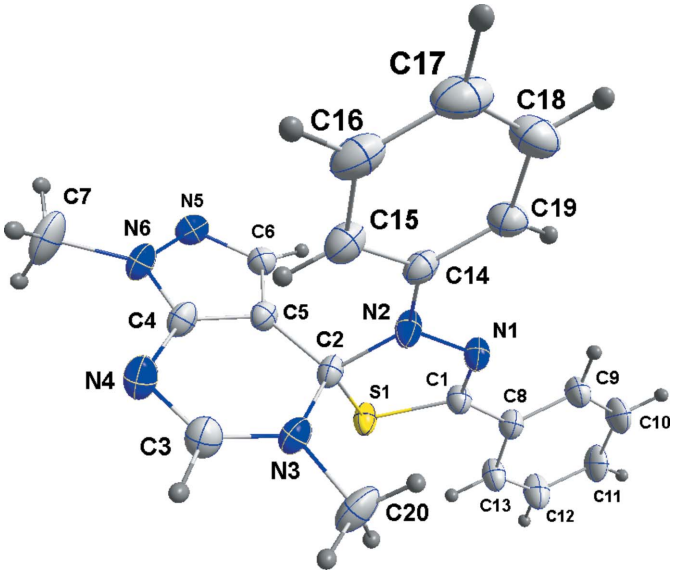


Figure 1
The S1-containing molecule, with the atom-labelling scheme and 50% probability displacement ellipsoids.

In the crystal, several C—H···N hydrogen bonds (Table 2) bind the molecules into double chains running along the *a*-axis direction (Fig. 3). An end view of the chains (Fig. 4) shows them to have their hydrophobic portions on the outside surfaces of the chains.

Synthesis and crystallization

Triethylamine (2 ml) was added to a solution of 1,5-dimethyl-1*H*-pyrazolo[3,4-*d*]pyrimidin-4(5*H*)-thione (2 g, 10 mmol) and diphenyl hydrazonoyl chloride (3.00 g, 13 mmol) in tetrahydrofuran (THF, 30 ml). The mixture was refluxed for 24 h. The precipitate was collected by filtration and separated by silica-gel chromatography (hexane–ethyl acetate 8:2 *v*/*v*). The solid obtained was recrystallized from ethanol solution to afford the title compound as yellow crystals (yield 70%).

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···N11^{i}	0.95	2.49	3.247 (5)	137
C7—H7*C*···N22	0.98	2.49	3.382 (6)	151
C23—H23···N5	0.95	2.41	3.232 (5)	144
C43—H43···N23^{ii}	0.95	2.60	3.286 (5)	129
C59—H59···N15	0.95	2.56	3.144 (5)	120
C63—H63···N17	0.95	2.53	3.284 (5)	137
C67—H67*C*···N4	0.98	2.57	3.472 (6)	153
C79—H79···N21	0.95	2.54	3.140 (5)	121

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

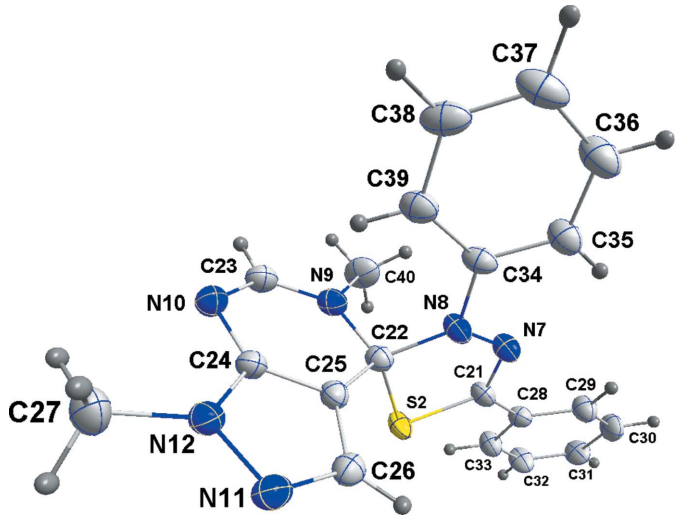


Figure 2
The S2-containing molecule, with the atom-labelling scheme and 50% probability displacement ellipsoids.

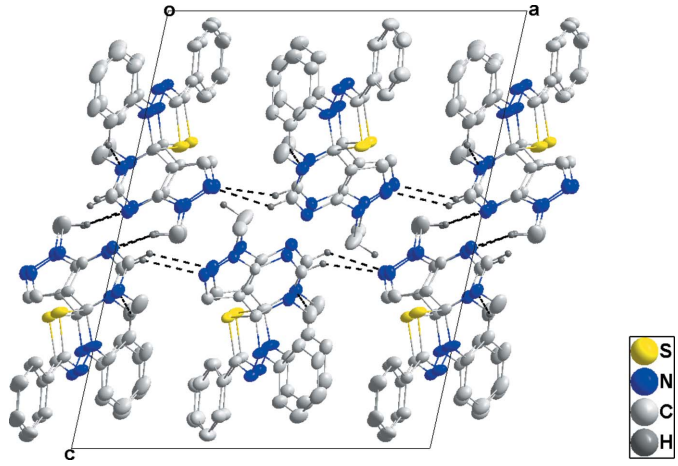


Figure 3
Packing viewed along the *b*-axis direction, showing one of the double chains formed by C—H···N hydrogen bonds.

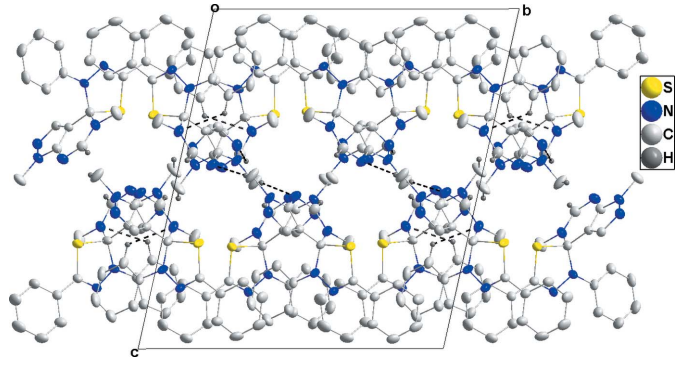


Figure 4
Packing viewed along the *a*-axis direction, showing an end view of two adjacent double chains.

Refinement

Crystal and refinement details are presented in Table 3. Refined as a two-component twin.

Acknowledgements

The support of the Tulane Crystallography Laboratory by Tulane University is gratefully acknowledged.

Funding information

Funding for this research was provided by: National Science Foundation Major Research Instrumentation (NSF-MRI) Program (grant No. 1228232).

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Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{18}N_6S$
M_r	374.46
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	150
a, b, c (Å)	14.0103 (6), 15.4161 (7), 17.9614 (8)
α, β, γ (°)	102.333 (2), 102.133 (2), 90.195 (2)
V (Å^3)	3700.5 (3)
Z	8
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.69
Crystal size (mm)	0.21 × 0.13 × 0.10
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*TWINABS*; Sheldrick, 2009)
T_{min}, T_{max}	0.72, 0.85
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	82602, 82602, 57463
R_{int}	? **PLEASE SUPPLY**
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.618
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.054, 0.140, 1.02
No. of reflections	82602
No. of parameters	982
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.24, −0.42

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

full crystallographic data

IUCrData (2017). **2**, x171042 [https://doi.org/10.1107/S2414314617010422]

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1,5-Dimethyl-3′,5′-diphenyl-1,5-dihydro-3′*H*-spiro[pyrazolo[3,4-*d*]pyrimidine-4,2′-[1,3,4]-thiadiazole]

Crystal data

$C_{20}H_{18}N_6S$
M_r = 374.46
Triclinic, $P\overline{1}$
a = 14.0103 (6) Å
b = 15.4161 (7) Å
c = 17.9614 (8) Å
α = 102.333 (2)°
β = 102.133 (2)°
γ = 90.195 (2)°
V = 3700.5 (3) Å^3
Z = 8
$F(000)$ = 1568
D_x = 1.344 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9980 reflections
θ = 2.9–72.3°
μ = 1.69 mm^{-1}
T = 150 K
Block, colourless
0.21 × 0.13 × 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 (*TWINABS*; Sheldrick, 2009)
T_{min} = 0.72, T_{max} = 0.85
82602 measured reflections
82602 independent reflections
57463 reflections with $I > 2\sigma(I)$
θ_{max} = 72.4°, θ_{min} = 2.9°
h = −17→17
k = −19→19
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.140
S = 1.02
82602 reflections
982 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
$w = 1/[\sigma^2(F_o^2) + (0.0572P)^2 + 0.2552P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Special details

Experimental. Analysis of 3339 reflections having I/σ(I) > 12 and chosen from the full data set with *CELL_NOW* (Sheldrick, 2008) showed the crystal to belong to the triclinic system and to be twinned by a 180° rotation about the *b* axis. The raw data were processed using the multi-component version of *SAINT* under control of the two-component orientation file generated by *CELL_NOW*.

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) and included as riding contributions with isotropic displacement parameters 1.2 - 1.5 times those of the attached atoms. Refined as a 2-component twin.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.85636 (7)	0.62142 (6)	0.69935 (5)	0.0277 (2)
N1	0.9579 (3)	0.5987 (2)	0.83082 (18)	0.0267 (7)
N2	0.9700 (3)	0.5236 (2)	0.77714 (18)	0.0304 (7)
N3	1.0125 (2)	0.5337 (2)	0.65400 (19)	0.0285 (7)
N4	0.9770 (3)	0.4030 (2)	0.55149 (19)	0.0313 (7)
N5	0.7630 (3)	0.3261 (3)	0.5985 (2)	0.0299 (7)
N6	0.8326 (3)	0.3205 (3)	0.5563 (2)	0.0285 (7)
C1	0.9031 (3)	0.6547 (3)	0.8008 (2)	0.0249 (8)
C2	0.9336 (3)	0.5227 (3)	0.6934 (2)	0.0244 (7)
C3	1.0281 (3)	0.4760 (3)	0.5894 (2)	0.0304 (8)
H3	1.0824	0.4905	0.5696	0.036*
C4	0.9000 (3)	0.3893 (3)	0.5838 (2)	0.0258 (7)
C5	0.8735 (3)	0.4411 (3)	0.6479 (2)	0.0233 (7)
C6	0.7874 (3)	0.4003 (3)	0.6542 (2)	0.0264 (7)
H6	0.7510	0.4223	0.6928	0.032*
C7	0.8301 (4)	0.2469 (4)	0.4901 (3)	0.0471 (11)
H7A	0.8046	0.2665	0.4416	0.071*
H7B	0.7876	0.1980	0.4937	0.071*
H7C	0.8963	0.2265	0.4904	0.071*
C8	0.8772 (3)	0.7379 (3)	0.8467 (2)	0.0260 (8)
C9	0.8917 (3)	0.7496 (3)	0.9280 (2)	0.0308 (9)
H9	0.9182	0.7040	0.9531	0.037*
C10	0.8667 (4)	0.8289 (3)	0.9711 (2)	0.0377 (10)
H10	0.8765	0.8374	1.0262	0.045*
C11	0.8284 (4)	0.8948 (3)	0.9356 (3)	0.0378 (10)
H11	0.8120	0.9488	0.9659	0.045*
C12	0.8133 (4)	0.8826 (3)	0.8549 (3)	0.0399 (10)
H12	0.7859	0.9281	0.8300	0.048*
C13	0.8380 (4)	0.8050 (4)	0.8112 (2)	0.0321 (9)
H13	0.8282	0.7972	0.7562	0.039*

C14	1.0324 (3)	0.4608 (3)	0.8056 (2)	0.0270 (8)
C15	1.0704 (3)	0.3934 (3)	0.7558 (2)	0.0311 (8)
H15	1.0545	0.3888	0.7009	0.037*
C16	1.1318 (3)	0.3333 (3)	0.7873 (3)	0.0363 (9)
H16	1.1579	0.2881	0.7535	0.044*
C17	1.1553 (4)	0.3384 (3)	0.8663 (3)	0.0423 (10)
H17	1.1973	0.2970	0.8870	0.051*
C18	1.1177 (4)	0.4036 (3)	0.9151 (3)	0.0434 (10)
H18	1.1337	0.4070	0.9697	0.052*
C19	1.0562 (3)	0.4653 (3)	0.8857 (2)	0.0332 (8)
H19	1.0307	0.5101	0.9202	0.040*
C20	1.0796 (3)	0.6109 (3)	0.6878 (3)	0.0429 (10)
H20A	1.1325	0.6080	0.6595	0.064*
H20B	1.1070	0.6116	0.7428	0.064*
H20C	1.0444	0.6651	0.6838	0.064*
S2	0.35732 (8)	0.23263 (7)	0.70015 (5)	0.0279 (2)
N7	0.4567 (3)	0.3193 (2)	0.83337 (18)	0.0281 (7)
N8	0.4667 (2)	0.3708 (2)	0.78165 (17)	0.0287 (6)
N9	0.5143 (2)	0.3038 (2)	0.65920 (18)	0.0289 (7)
N10	0.4816 (2)	0.3863 (2)	0.55894 (17)	0.0310 (7)
N11	0.2630 (3)	0.4799 (2)	0.6033 (2)	0.0276 (7)
N12	0.3347 (2)	0.4672 (2)	0.56161 (18)	0.0272 (7)
C21	0.4030 (3)	0.2485 (3)	0.8014 (2)	0.0255 (8)
C22	0.4325 (3)	0.3313 (3)	0.6970 (2)	0.0253 (7)
C23	0.5319 (3)	0.3319 (2)	0.5966 (2)	0.0296 (7)
H23	0.5875	0.3092	0.5779	0.036*
C24	0.4016 (3)	0.4127 (2)	0.5898 (2)	0.0242 (7)
C25	0.3740 (3)	0.3897 (2)	0.6525 (2)	0.0230 (7)
C26	0.2869 (3)	0.4323 (3)	0.6573 (2)	0.0252 (7)
H26	0.2494	0.4278	0.6948	0.030*
C27	0.3339 (3)	0.5111 (3)	0.4977 (2)	0.0394 (9)
H27A	0.3863	0.4893	0.4711	0.059*
H27B	0.3441	0.5754	0.5181	0.059*
H27C	0.2707	0.4982	0.4607	0.059*
C28	0.3796 (3)	0.1849 (3)	0.8459 (2)	0.0248 (8)
C29	0.3911 (3)	0.2092 (3)	0.9263 (2)	0.0320 (9)
H29	0.4146	0.2680	0.9527	0.038*
C30	0.3693 (4)	0.1502 (3)	0.9690 (2)	0.0369 (9)
H30	0.3784	0.1680	1.0241	0.044*
C31	0.3336 (3)	0.0634 (3)	0.9300 (3)	0.0357 (9)
H31	0.3181	0.0223	0.9588	0.043*
C32	0.3211 (4)	0.0381 (3)	0.8504 (3)	0.0363 (9)
H32	0.2969	−0.0205	0.8242	0.044*
C33	0.3440 (4)	0.0983 (3)	0.8077 (2)	0.0315 (9)
H33	0.3353	0.0804	0.7527	0.038*
C34	0.5301 (3)	0.4479 (2)	0.8123 (2)	0.0267 (7)
C35	0.5523 (3)	0.4812 (3)	0.8930 (2)	0.0332 (8)
H35	0.5249	0.4523	0.9260	0.040*

C36	0.6140 (3)	0.5559 (3)	0.9250 (2)	0.0419 (9)
H36	0.6281	0.5779	0.9800	0.050*
C37	0.6559 (3)	0.5998 (3)	0.8786 (2)	0.0428 (10)
H37	0.6989	0.6507	0.9011	0.051*
C38	0.6330 (3)	0.5669 (3)	0.7988 (2)	0.0352 (8)
H38	0.6606	0.5961	0.7662	0.042*
C39	0.5704 (3)	0.4917 (2)	0.7649 (2)	0.0306 (7)
H39	0.5553	0.4706	0.7099	0.037*
C40	0.5820 (3)	0.2433 (3)	0.6938 (3)	0.0444 (10)
H40A	0.5470	0.1866	0.6892	0.067*
H40B	0.6084	0.2699	0.7490	0.067*
H40C	0.6358	0.2330	0.6663	0.067*
S3	0.62544 (9)	0.27527 (7)	0.30929 (5)	0.0334 (2)
N13	0.5245 (3)	0.1806 (2)	0.17985 (18)	0.0286 (7)
N14	0.5087 (3)	0.1380 (2)	0.23570 (17)	0.0362 (8)
N15	0.4718 (2)	0.2129 (2)	0.36022 (19)	0.0312 (7)
N16	0.5122 (2)	0.1395 (2)	0.46584 (17)	0.0328 (7)
N17	0.7188 (3)	0.0312 (3)	0.4112 (2)	0.0366 (8)
N18	0.6536 (2)	0.0513 (2)	0.45801 (19)	0.0320 (7)
C41	0.5820 (3)	0.2500 (3)	0.2074 (2)	0.0273 (8)
C42	0.5491 (3)	0.1804 (3)	0.3191 (2)	0.0292 (8)
C43	0.4599 (3)	0.1912 (3)	0.4269 (2)	0.0318 (8)
H43	0.4069	0.2167	0.4478	0.038*
C44	0.5868 (3)	0.1068 (3)	0.4309 (2)	0.0272 (8)
C45	0.6081 (3)	0.1228 (3)	0.3635 (2)	0.0261 (8)
C46	0.6919 (3)	0.0746 (3)	0.3546 (2)	0.0313 (8)
H46	0.7248	0.0734	0.3133	0.038*
C47	0.6592 (4)	0.0130 (4)	0.5255 (3)	0.0538 (13)
H47A	0.6412	−0.0508	0.5083	0.081*
H47B	0.6141	0.0420	0.5568	0.081*
H47C	0.7260	0.0216	0.5571	0.081*
C48	0.6126 (3)	0.3048 (3)	0.1584 (2)	0.0254 (8)
C49	0.6604 (4)	0.3877 (3)	0.1918 (3)	0.0331 (10)
H49	0.6719	0.4096	0.2467	0.040*
C50	0.6915 (4)	0.4391 (3)	0.1451 (3)	0.0412 (11)
H50	0.7238	0.4957	0.1681	0.049*
C51	0.6753 (4)	0.4072 (3)	0.0660 (3)	0.0435 (11)
H51	0.6966	0.4418	0.0341	0.052*
C52	0.6274 (4)	0.3240 (3)	0.0318 (2)	0.0403 (10)
H52	0.6157	0.3023	−0.0231	0.048*
C53	0.5971 (3)	0.2734 (3)	0.0782 (2)	0.0356 (9)
H53	0.5653	0.2166	0.0550	0.043*
C54	0.4513 (3)	0.0574 (3)	0.2101 (2)	0.0273 (7)
C55	0.4342 (3)	0.0145 (3)	0.1314 (2)	0.0311 (8)
H55	0.4618	0.0393	0.0961	0.037*
C56	0.3773 (3)	−0.0637 (3)	0.1046 (2)	0.0391 (9)
H56	0.3662	−0.0920	0.0509	0.047*
C57	0.3358 (3)	−0.1020 (3)	0.1546 (2)	0.0366 (8)

H57	0.2968	−0.1559	0.1358	0.044*
C58	0.3530 (3)	−0.0592 (2)	0.2326 (2)	0.0314 (7)
H58	0.3249	−0.0841	0.2675	0.038*
C59	0.4106 (3)	0.0194 (2)	0.2609 (2)	0.0294 (7)
H59	0.4221	0.0472	0.3147	0.035*
C60	0.4038 (3)	0.2736 (3)	0.3258 (3)	0.0506 (12)
H60A	0.3780	0.2474	0.2703	0.076*
H60B	0.4385	0.3307	0.3311	0.076*
H60C	0.3497	0.2832	0.3529	0.076*
S4	1.11811 (8)	−0.12100 (7)	0.31088 (5)	0.0350 (2)
N19	1.0224 (3)	−0.0938 (3)	0.17908 (19)	0.0311 (7)
N20	1.0043 (3)	−0.0223 (2)	0.23337 (18)	0.0381 (9)
N21	0.9678 (3)	−0.0263 (2)	0.3594 (2)	0.0332 (7)
N22	1.0099 (3)	0.1071 (2)	0.45857 (19)	0.0330 (7)
N23	1.2207 (3)	0.1751 (3)	0.4012 (2)	0.0320 (7)
N24	1.1541 (3)	0.1844 (3)	0.4465 (2)	0.0306 (7)
C61	1.0771 (3)	−0.1501 (3)	0.2086 (2)	0.0268 (8)
C62	1.0448 (3)	−0.0197 (3)	0.3170 (2)	0.0287 (8)
C63	0.9561 (3)	0.0344 (3)	0.4235 (2)	0.0333 (8)
H63	0.9026	0.0227	0.4454	0.040*
C64	1.0852 (3)	0.1167 (3)	0.4234 (2)	0.0265 (8)
C65	1.1074 (3)	0.0616 (3)	0.3588 (2)	0.0257 (8)
C66	1.1924 (3)	0.0995 (3)	0.3478 (2)	0.0302 (8)
H66	1.2258	0.0751	0.3079	0.036*
C67	1.1605 (4)	0.2614 (4)	0.5106 (3)	0.0475 (11)
H67A	1.2024	0.3085	0.5033	0.071*
H67B	1.1883	0.2445	0.5600	0.071*
H67C	1.0950	0.2830	0.5118	0.071*
C68	1.1086 (3)	−0.2294 (3)	0.1619 (2)	0.0267 (8)
C69	1.1537 (4)	−0.2956 (4)	0.1961 (2)	0.0331 (9)
H69	1.1634	−0.2899	0.2509	0.040*
C70	1.1843 (4)	−0.3692 (3)	0.1512 (3)	0.0393 (10)
H70	1.2159	−0.4139	0.1752	0.047*
C71	1.1694 (4)	−0.3789 (3)	0.0708 (3)	0.0396 (10)
H71	1.1896	−0.4305	0.0398	0.048*
C72	1.1258 (4)	−0.3140 (4)	0.0366 (2)	0.0405 (10)
H72	1.1164	−0.3206	−0.0183	0.049*
C73	1.0950 (3)	−0.2388 (3)	0.0808 (2)	0.0326 (9)
H73	1.0649	−0.1939	0.0564	0.039*
C74	0.9507 (3)	0.0454 (3)	0.2048 (2)	0.0304 (8)
C75	0.9390 (3)	0.0472 (3)	0.1264 (3)	0.0357 (9)
H75	0.9683	0.0041	0.0930	0.043*
C76	0.8839 (4)	0.1126 (3)	0.0966 (3)	0.0436 (10)
H76	0.8762	0.1138	0.0430	0.052*
C77	0.8407 (4)	0.1751 (3)	0.1441 (3)	0.0440 (10)
H77	0.8030	0.2189	0.1233	0.053*
C78	0.8523 (3)	0.1739 (3)	0.2214 (3)	0.0376 (9)
H78	0.8222	0.2170	0.2541	0.045*

C79	0.9078 (3)	0.1103 (3)	0.2529 (2)	0.0338 (8)
H79	0.9165	0.1110	0.3070	0.041*
C80	0.8989 (3)	−0.1028 (3)	0.3299 (3)	0.0489 (11)
H80A	0.8729	−0.1082	0.2739	0.073*
H80B	0.8451	−0.0949	0.3575	0.073*
H80C	0.9322	−0.1567	0.3384	0.073*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0317 (4)	0.0251 (4)	0.0214 (4)	0.0086 (3)	−0.0013 (3)	0.0012 (3)
N1	0.0281 (15)	0.0252 (14)	0.0223 (12)	0.0057 (11)	0.0003 (10)	0.0004 (11)
N2	0.0362 (16)	0.0234 (13)	0.0243 (13)	0.0090 (11)	−0.0040 (11)	−0.0007 (11)
N3	0.0250 (14)	0.0248 (13)	0.0313 (14)	−0.0024 (11)	0.0025 (11)	0.0002 (11)
N4	0.0214 (14)	0.0351 (15)	0.0326 (14)	−0.0008 (11)	0.0073 (11)	−0.0045 (12)
N5	0.0234 (15)	0.0273 (15)	0.0376 (15)	0.0011 (11)	0.0037 (11)	0.0070 (12)
N6	0.0216 (14)	0.0236 (13)	0.0336 (14)	0.0002 (11)	0.0028 (11)	−0.0049 (12)
C1	0.0262 (17)	0.0239 (16)	0.0224 (15)	0.0047 (13)	0.0018 (12)	0.0037 (13)
C2	0.0243 (16)	0.0216 (14)	0.0225 (14)	0.0029 (12)	−0.0005 (11)	−0.0001 (11)
C3	0.0232 (16)	0.0331 (17)	0.0331 (16)	0.0025 (12)	0.0068 (12)	0.0025 (14)
C4	0.0209 (16)	0.0229 (15)	0.0284 (15)	0.0013 (12)	0.0008 (12)	−0.0009 (13)
C5	0.0219 (16)	0.0233 (15)	0.0222 (14)	0.0011 (12)	−0.0002 (11)	0.0042 (12)
C6	0.0256 (17)	0.0270 (15)	0.0268 (15)	0.0042 (13)	0.0055 (12)	0.0065 (13)
C7	0.034 (2)	0.035 (2)	0.057 (2)	0.0003 (16)	0.0044 (17)	−0.0201 (18)
C8	0.0228 (17)	0.0263 (17)	0.0259 (16)	0.0040 (13)	0.0024 (13)	0.0023 (14)
C9	0.035 (2)	0.0317 (18)	0.0235 (16)	0.0058 (14)	0.0038 (13)	0.0038 (14)
C10	0.040 (2)	0.045 (2)	0.0245 (16)	0.0099 (16)	0.0079 (14)	−0.0007 (15)
C11	0.0348 (19)	0.0402 (19)	0.0307 (18)	0.0126 (15)	0.0042 (14)	−0.0065 (14)
C12	0.045 (2)	0.036 (2)	0.0331 (18)	0.0161 (16)	−0.0004 (16)	0.0054 (16)
C13	0.038 (2)	0.0316 (19)	0.0233 (16)	0.0121 (16)	0.0025 (15)	0.0034 (15)
C14	0.0233 (16)	0.0206 (15)	0.0324 (16)	−0.0003 (12)	−0.0030 (12)	0.0048 (13)
C15	0.0279 (17)	0.0242 (16)	0.0368 (17)	0.0018 (13)	0.0001 (13)	0.0038 (13)
C16	0.0315 (19)	0.0228 (15)	0.052 (2)	0.0029 (13)	0.0027 (15)	0.0082 (14)
C17	0.037 (2)	0.0298 (18)	0.059 (2)	0.0080 (15)	−0.0032 (17)	0.0194 (17)
C18	0.047 (2)	0.041 (2)	0.042 (2)	0.0065 (17)	−0.0010 (16)	0.0220 (17)
C19	0.0366 (19)	0.0271 (16)	0.0354 (18)	0.0054 (14)	0.0023 (14)	0.0112 (14)
C20	0.0300 (19)	0.0314 (18)	0.058 (2)	−0.0098 (15)	0.0033 (16)	−0.0032 (16)
S2	0.0329 (4)	0.0259 (4)	0.0220 (4)	−0.0084 (3)	−0.0023 (3)	0.0073 (3)
N7	0.0346 (16)	0.0227 (13)	0.0257 (13)	−0.0055 (11)	0.0003 (11)	0.0090 (11)
N8	0.0349 (16)	0.0262 (13)	0.0228 (13)	−0.0098 (11)	−0.0022 (11)	0.0092 (11)
N9	0.0249 (14)	0.0292 (14)	0.0332 (15)	0.0048 (11)	0.0023 (11)	0.0123 (12)
N10	0.0245 (14)	0.0407 (16)	0.0311 (15)	0.0040 (12)	0.0074 (11)	0.0138 (12)
N11	0.0226 (14)	0.0294 (15)	0.0326 (14)	0.0028 (11)	0.0075 (11)	0.0093 (12)
N12	0.0222 (14)	0.0325 (16)	0.0296 (14)	0.0017 (11)	0.0038 (11)	0.0146 (12)
C21	0.0254 (17)	0.0255 (16)	0.0229 (15)	0.0006 (13)	−0.0007 (12)	0.0055 (13)
C22	0.0249 (16)	0.0241 (15)	0.0260 (16)	−0.0019 (12)	0.0024 (12)	0.0068 (12)
C23	0.0230 (15)	0.0333 (17)	0.0326 (17)	0.0024 (12)	0.0056 (12)	0.0076 (14)
C24	0.0188 (15)	0.0292 (16)	0.0253 (15)	0.0008 (12)	0.0031 (12)	0.0092 (13)

C25	0.0233 (16)	0.0233 (15)	0.0215 (14)	−0.0017 (12)	0.0022 (11)	0.0053 (12)
C26	0.0254 (17)	0.0242 (15)	0.0254 (15)	−0.0005 (12)	0.0058 (12)	0.0041 (12)
C27	0.036 (2)	0.052 (2)	0.0382 (19)	0.0089 (17)	0.0070 (16)	0.0283 (18)
C28	0.0225 (17)	0.0253 (17)	0.0255 (16)	−0.0006 (13)	0.0014 (13)	0.0071 (14)
C29	0.036 (2)	0.0293 (18)	0.0290 (17)	−0.0041 (14)	0.0050 (14)	0.0055 (14)
C30	0.042 (2)	0.045 (2)	0.0262 (16)	−0.0037 (17)	0.0073 (14)	0.0116 (16)
C31	0.039 (2)	0.035 (2)	0.0374 (18)	−0.0084 (15)	0.0095 (15)	0.0162 (15)
C32	0.043 (2)	0.0288 (18)	0.0361 (18)	−0.0122 (16)	0.0031 (15)	0.0107 (15)
C33	0.038 (2)	0.0283 (19)	0.0267 (17)	−0.0059 (15)	0.0021 (15)	0.0079 (15)
C34	0.0248 (16)	0.0202 (14)	0.0322 (18)	−0.0038 (12)	−0.0009 (13)	0.0064 (13)
C35	0.0382 (19)	0.0266 (16)	0.0310 (18)	−0.0034 (13)	0.0020 (14)	0.0033 (14)
C36	0.051 (2)	0.0293 (17)	0.038 (2)	−0.0101 (15)	−0.0004 (17)	0.0004 (16)
C37	0.042 (2)	0.0263 (17)	0.051 (2)	−0.0100 (15)	−0.0036 (18)	0.0034 (17)
C38	0.0281 (17)	0.0272 (16)	0.052 (2)	−0.0038 (13)	0.0030 (16)	0.0174 (17)
C39	0.0284 (17)	0.0280 (16)	0.0342 (17)	−0.0027 (13)	−0.0003 (13)	0.0112 (14)
C40	0.035 (2)	0.048 (2)	0.057 (2)	0.0117 (17)	0.0066 (17)	0.029 (2)
S3	0.0419 (5)	0.0323 (4)	0.0221 (4)	−0.0152 (4)	−0.0034 (3)	0.0082 (3)
N13	0.0343 (16)	0.0286 (14)	0.0219 (13)	−0.0074 (12)	0.0008 (11)	0.0084 (11)
N14	0.049 (2)	0.0347 (15)	0.0205 (13)	−0.0184 (14)	−0.0045 (12)	0.0086 (12)
N15	0.0289 (15)	0.0303 (15)	0.0334 (15)	0.0016 (12)	−0.0004 (11)	0.0120 (13)
N16	0.0269 (14)	0.0450 (17)	0.0284 (14)	−0.0002 (12)	0.0051 (11)	0.0132 (13)
N17	0.0295 (17)	0.0282 (15)	0.0497 (19)	0.0004 (13)	0.0018 (14)	0.0100 (14)
N18	0.0264 (15)	0.0337 (15)	0.0358 (16)	−0.0026 (12)	−0.0028 (12)	0.0166 (13)
C41	0.0294 (18)	0.0282 (17)	0.0224 (15)	−0.0034 (13)	−0.0008 (12)	0.0076 (13)
C42	0.035 (2)	0.0295 (16)	0.0198 (15)	−0.0079 (14)	−0.0015 (13)	0.0051 (13)
C43	0.0244 (16)	0.0369 (18)	0.0332 (17)	−0.0003 (13)	0.0048 (13)	0.0070 (14)
C44	0.0246 (17)	0.0302 (17)	0.0247 (15)	−0.0047 (13)	−0.0027 (12)	0.0091 (13)
C45	0.0263 (17)	0.0251 (15)	0.0232 (15)	−0.0044 (13)	−0.0001 (12)	0.0029 (13)
C46	0.031 (2)	0.0267 (16)	0.0327 (17)	−0.0043 (15)	0.0061 (14)	−0.0009 (14)
C47	0.041 (2)	0.069 (3)	0.055 (3)	−0.009 (2)	−0.0117 (19)	0.045 (2)
C48	0.0228 (17)	0.0270 (18)	0.0259 (16)	−0.0012 (13)	0.0018 (13)	0.0078 (14)
C49	0.039 (2)	0.033 (2)	0.0277 (18)	−0.0052 (16)	0.0057 (16)	0.0090 (15)
C50	0.045 (2)	0.043 (2)	0.0384 (19)	−0.0121 (18)	0.0105 (17)	0.0130 (18)
C51	0.040 (2)	0.059 (3)	0.039 (2)	−0.006 (2)	0.0114 (16)	0.023 (2)
C52	0.043 (2)	0.052 (2)	0.0256 (17)	−0.0082 (18)	0.0074 (15)	0.0083 (17)
C53	0.036 (2)	0.042 (2)	0.0272 (17)	−0.0036 (16)	0.0043 (14)	0.0076 (16)
C54	0.0270 (17)	0.0232 (15)	0.0280 (16)	−0.0020 (12)	−0.0025 (12)	0.0059 (14)
C55	0.0338 (18)	0.0278 (16)	0.0301 (18)	0.0005 (13)	0.0034 (14)	0.0061 (14)
C56	0.047 (2)	0.0277 (17)	0.036 (2)	−0.0016 (15)	0.0031 (16)	−0.0019 (16)
C57	0.0358 (19)	0.0233 (15)	0.049 (2)	−0.0034 (13)	0.0059 (16)	0.0069 (16)
C58	0.0281 (16)	0.0254 (15)	0.0409 (19)	0.0016 (12)	0.0033 (14)	0.0119 (14)
C59	0.0306 (17)	0.0256 (15)	0.0299 (16)	−0.0006 (12)	0.0006 (13)	0.0079 (13)
C60	0.038 (2)	0.044 (2)	0.071 (3)	0.0075 (18)	−0.0023 (19)	0.028 (2)
S4	0.0460 (6)	0.0280 (4)	0.0224 (4)	0.0148 (4)	−0.0053 (3)	−0.0009 (3)
N19	0.0377 (18)	0.0255 (14)	0.0232 (13)	0.0049 (12)	−0.0023 (11)	−0.0008 (12)
N20	0.052 (2)	0.0275 (14)	0.0231 (14)	0.0165 (14)	−0.0084 (13)	−0.0033 (11)
N21	0.0299 (16)	0.0250 (13)	0.0374 (16)	−0.0020 (12)	−0.0025 (12)	0.0007 (12)
N22	0.0265 (15)	0.0331 (14)	0.0335 (14)	−0.0005 (11)	0.0057 (11)	−0.0046 (12)

N23	0.0258 (16)	0.0305 (16)	0.0408 (16)	0.0045 (12)	0.0089 (12)	0.0086 (13)
N24	0.0253 (15)	0.0256 (14)	0.0340 (14)	0.0000 (11)	0.0022 (11)	−0.0045 (12)
C61	0.0289 (19)	0.0255 (16)	0.0228 (15)	0.0015 (13)	−0.0017 (13)	0.0052 (13)
C62	0.0296 (19)	0.0246 (15)	0.0249 (15)	0.0052 (14)	−0.0043 (13)	0.0003 (12)
C63	0.0259 (17)	0.0326 (17)	0.0386 (18)	0.0010 (13)	0.0052 (13)	0.0036 (14)
C64	0.0215 (16)	0.0253 (15)	0.0289 (15)	0.0028 (12)	0.0028 (12)	0.0003 (12)
C65	0.0285 (18)	0.0239 (15)	0.0212 (14)	0.0067 (13)	0.0009 (12)	0.0020 (12)
C66	0.033 (2)	0.0304 (17)	0.0298 (16)	0.0102 (15)	0.0095 (13)	0.0093 (14)
C67	0.039 (2)	0.036 (2)	0.054 (2)	−0.0047 (17)	0.0087 (18)	−0.0175 (18)
C68	0.0257 (18)	0.0274 (17)	0.0241 (16)	0.0004 (14)	0.0032 (13)	0.0019 (14)
C69	0.039 (2)	0.034 (2)	0.0256 (17)	0.0107 (16)	0.0047 (15)	0.0061 (15)
C70	0.047 (2)	0.0333 (19)	0.0352 (19)	0.0161 (16)	0.0075 (16)	0.0036 (16)
C71	0.039 (2)	0.041 (2)	0.0340 (19)	0.0146 (16)	0.0105 (15)	−0.0041 (16)
C72	0.044 (2)	0.052 (2)	0.0227 (16)	0.0085 (18)	0.0097 (15)	−0.0011 (16)
C73	0.035 (2)	0.0360 (19)	0.0245 (16)	0.0060 (15)	0.0033 (14)	0.0052 (14)
C74	0.0284 (18)	0.0208 (15)	0.0342 (17)	0.0014 (13)	−0.0076 (13)	0.0028 (13)
C75	0.039 (2)	0.0288 (17)	0.0381 (19)	0.0018 (14)	0.0006 (15)	0.0115 (15)
C76	0.049 (2)	0.036 (2)	0.046 (2)	0.0057 (17)	0.0011 (17)	0.0203 (17)
C77	0.039 (2)	0.0309 (18)	0.061 (2)	0.0043 (15)	−0.0044 (17)	0.0209 (18)
C78	0.0276 (18)	0.0207 (15)	0.060 (2)	0.0024 (13)	0.0005 (15)	0.0072 (15)
C79	0.0312 (19)	0.0243 (15)	0.0392 (18)	0.0035 (13)	−0.0032 (14)	0.0028 (14)
C80	0.041 (2)	0.0290 (17)	0.062 (3)	−0.0066 (16)	−0.0064 (19)	−0.0046 (18)

Geometric parameters (Å, º)

S1—C1	1.763 (4)	S3—C41	1.760 (4)
S1—C2	1.868 (4)	S3—C42	1.869 (4)
N1—C1	1.286 (6)	N13—C41	1.280 (6)
N1—N2	1.376 (5)	N13—N14	1.364 (4)
N2—C14	1.412 (5)	N14—C54	1.412 (5)
N2—C2	1.480 (5)	N14—C42	1.488 (4)
N3—C3	1.361 (5)	N15—C43	1.353 (5)
N3—C20	1.453 (5)	N15—C42	1.467 (5)
N3—C2	1.460 (4)	N15—C60	1.475 (6)
N4—C3	1.305 (5)	N16—C43	1.298 (5)
N4—C4	1.364 (5)	N16—C44	1.374 (5)
N5—C6	1.339 (6)	N17—C46	1.325 (6)
N5—N6	1.348 (5)	N17—N18	1.361 (5)
N6—C4	1.355 (5)	N18—C44	1.354 (5)
N6—C7	1.452 (6)	N18—C47	1.446 (5)
C1—C8	1.461 (6)	C41—C48	1.465 (5)
C2—C5	1.491 (5)	C42—C45	1.462 (6)
C3—H3	0.9500	C43—H43	0.9500
C4—C5	1.374 (5)	C44—C45	1.376 (5)
C5—C6	1.396 (5)	C45—C46	1.411 (5)
C6—H6	0.9500	C46—H46	0.9500
C7—H7A	0.9800	C47—H47A	0.9800
C7—H7B	0.9800	C47—H47B	0.9800

C7—H7C	0.9800	C47—H47C	0.9800
C8—C13	1.385 (7)	C48—C53	1.389 (6)
C8—C9	1.402 (5)	C48—C49	1.393 (7)
C9—C10	1.388 (6)	C49—C50	1.398 (6)
C9—H9	0.9500	C49—H49	0.9500
C10—C11	1.365 (7)	C50—C51	1.371 (7)
C10—H10	0.9500	C50—H50	0.9500
C11—C12	1.391 (6)	C51—C52	1.399 (7)
C11—H11	0.9500	C51—H51	0.9500
C12—C13	1.372 (7)	C52—C53	1.380 (6)
C12—H12	0.9500	C52—H52	0.9500
C13—H13	0.9500	C53—H53	0.9500
C14—C19	1.394 (5)	C54—C59	1.395 (5)
C14—C15	1.403 (5)	C54—C55	1.397 (5)
C15—C16	1.394 (6)	C55—C56	1.381 (6)
C15—H15	0.9500	C55—H55	0.9500
C16—C17	1.373 (6)	C56—C57	1.391 (5)
C16—H16	0.9500	C56—H56	0.9500
C17—C18	1.371 (7)	C57—C58	1.383 (5)
C17—H17	0.9500	C57—H57	0.9500
C18—C19	1.398 (6)	C58—C59	1.392 (5)
C18—H18	0.9500	C58—H58	0.9500
C19—H19	0.9500	C59—H59	0.9500
C20—H20A	0.9800	C60—H60A	0.9800
C20—H20B	0.9800	C60—H60B	0.9800
C20—H20C	0.9800	C60—H60C	0.9800
S2—C21	1.760 (4)	S4—C61	1.763 (4)
S2—C22	1.865 (4)	S4—C62	1.869 (4)
N7—C21	1.278 (6)	N19—C61	1.285 (6)
N7—N8	1.372 (4)	N19—N20	1.370 (5)
N8—C34	1.418 (5)	N20—C74	1.411 (5)
N8—C22	1.487 (4)	N20—C62	1.481 (5)
N9—C23	1.355 (5)	N21—C63	1.359 (5)
N9—C22	1.470 (4)	N21—C80	1.453 (6)
N9—C40	1.471 (5)	N21—C62	1.461 (5)
N10—C23	1.305 (5)	N22—C63	1.310 (5)
N10—C24	1.377 (4)	N22—C64	1.361 (5)
N11—C26	1.328 (6)	N23—C66	1.340 (6)
N11—N12	1.365 (4)	N23—N24	1.349 (5)
N12—C24	1.352 (5)	N24—C64	1.354 (6)
N12—C27	1.450 (5)	N24—C67	1.454 (6)
C21—C28	1.466 (6)	C61—C68	1.454 (6)
C22—C25	1.469 (5)	C62—C65	1.489 (6)
C23—H23	0.9500	C63—H63	0.9500
C24—C25	1.377 (5)	C64—C65	1.377 (5)
C25—C26	1.397 (5)	C65—C66	1.394 (6)
C26—H26	0.9500	C66—H66	0.9500
C27—H27A	0.9800	C67—H67A	0.9800

C27—H27B	0.9800	C67—H67B	0.9800
C27—H27C	0.9800	C67—H67C	0.9800
C28—C29	1.387 (6)	C68—C69	1.388 (7)
C28—C33	1.400 (6)	C68—C73	1.405 (5)
C29—C30	1.378 (6)	C69—C70	1.371 (7)
C29—H29	0.9500	C69—H69	0.9500
C30—C31	1.407 (6)	C70—C71	1.390 (7)
C30—H30	0.9500	C70—H70	0.9500
C31—C32	1.373 (6)	C71—C72	1.364 (7)
C31—H31	0.9500	C71—H71	0.9500
C32—C33	1.399 (6)	C72—C73	1.383 (6)
C32—H32	0.9500	C72—H72	0.9500
C33—H33	0.9500	C73—H73	0.9500
C34—C39	1.395 (5)	C74—C75	1.389 (6)
C34—C35	1.398 (5)	C74—C79	1.402 (6)
C35—C36	1.380 (6)	C75—C76	1.400 (7)
C35—H35	0.9500	C75—H75	0.9500
C36—C37	1.394 (6)	C76—C77	1.375 (7)
C36—H36	0.9500	C76—H76	0.9500
C37—C38	1.382 (6)	C77—C78	1.368 (7)
C37—H37	0.9500	C77—H77	0.9500
C38—C39	1.396 (5)	C78—C79	1.394 (6)
C38—H38	0.9500	C78—H78	0.9500
C39—H39	0.9500	C79—H79	0.9500
C40—H40A	0.9800	C80—H80A	0.9800
C40—H40B	0.9800	C80—H80B	0.9800
C40—H40C	0.9800	C80—H80C	0.9800

C1—S1—C2	91.05 (18)	C41—S3—C42	90.88 (18)
C1—N1—N2	113.5 (3)	C41—N13—N14	113.2 (3)
N1—N2—C14	116.5 (3)	N13—N14—C54	117.2 (3)
N1—N2—C2	117.9 (3)	N13—N14—C42	118.6 (3)
C14—N2—C2	124.4 (3)	C54—N14—C42	124.2 (3)
C3—N3—C20	118.5 (3)	C43—N15—C42	124.4 (3)
C3—N3—C2	124.5 (3)	C43—N15—C60	118.8 (3)
C20—N3—C2	117.0 (3)	C42—N15—C60	116.8 (3)
C3—N4—C4	111.4 (3)	C43—N16—C44	111.2 (3)
C6—N5—N6	105.3 (3)	C46—N17—N18	105.5 (3)
N5—N6—C4	111.9 (3)	C44—N18—N17	111.1 (3)
N5—N6—C7	120.8 (4)	C44—N18—C47	128.1 (4)
C4—N6—C7	127.3 (4)	N17—N18—C47	120.8 (4)
N1—C1—C8	123.3 (4)	N13—C41—C48	123.2 (4)
N1—C1—S1	114.8 (3)	N13—C41—S3	115.7 (3)
C8—C1—S1	121.8 (3)	C48—C41—S3	121.1 (3)
N3—C2—N2	112.4 (3)	C45—C42—N15	107.5 (3)
N3—C2—C5	107.5 (3)	C45—C42—N14	114.5 (3)
N2—C2—C5	114.5 (3)	N15—C42—N14	111.9 (3)
N3—C2—S1	111.0 (3)	C45—C42—S3	111.2 (3)

N2—C2—S1	101.1 (2)	N15—C42—S3	110.7 (3)
C5—C2—S1	110.3 (3)	N14—C42—S3	101.1 (2)
N4—C3—N3	127.6 (4)	N16—C43—N15	127.7 (3)
N4—C3—H3	116.2	N16—C43—H43	116.1
N3—C3—H3	116.2	N15—C43—H43	116.1
N6—C4—N4	125.1 (3)	N18—C44—N16	124.8 (3)
N6—C4—C5	106.5 (3)	N18—C44—C45	107.5 (4)
N4—C4—C5	128.3 (4)	N16—C44—C45	127.6 (4)
C4—C5—C6	105.6 (3)	C44—C45—C46	104.5 (4)
C4—C5—C2	120.7 (3)	C44—C45—C42	121.5 (4)
C6—C5—C2	133.7 (3)	C46—C45—C42	134.0 (3)
N5—C6—C5	110.7 (3)	N17—C46—C45	111.4 (3)
N5—C6—H6	124.7	N17—C46—H46	124.3
C5—C6—H6	124.7	C45—C46—H46	124.3
N6—C7—H7A	109.5	N18—C47—H47A	109.5
N6—C7—H7B	109.5	N18—C47—H47B	109.5
H7A—C7—H7B	109.5	H47A—C47—H47B	109.5
N6—C7—H7C	109.5	N18—C47—H47C	109.5
H7A—C7—H7C	109.5	H47A—C47—H47C	109.5
H7B—C7—H7C	109.5	H47B—C47—H47C	109.5
C13—C8—C9	119.6 (4)	C53—C48—C49	119.1 (4)
C13—C8—C1	121.0 (4)	C53—C48—C41	120.3 (4)
C9—C8—C1	119.4 (4)	C49—C48—C41	120.6 (4)
C10—C9—C8	118.9 (4)	C48—C49—C50	120.5 (4)
C10—C9—H9	120.5	C48—C49—H49	119.8
C8—C9—H9	120.5	C50—C49—H49	119.8
C11—C10—C9	121.1 (4)	C51—C50—C49	119.6 (5)
C11—C10—H10	119.5	C51—C50—H50	120.2
C9—C10—H10	119.5	C49—C50—H50	120.2
C10—C11—C12	119.8 (4)	C50—C51—C52	120.4 (4)
C10—C11—H11	120.1	C50—C51—H51	119.8
C12—C11—H11	120.1	C52—C51—H51	119.8
C13—C12—C11	120.1 (5)	C53—C52—C51	119.8 (4)
C13—C12—H12	119.9	C53—C52—H52	120.1
C11—C12—H12	119.9	C51—C52—H52	120.1
C12—C13—C8	120.4 (4)	C52—C53—C48	120.6 (4)
C12—C13—H13	119.8	C52—C53—H53	119.7
C8—C13—H13	119.8	C48—C53—H53	119.7
C19—C14—C15	118.9 (4)	C59—C54—C55	118.8 (3)
C19—C14—N2	118.9 (4)	C59—C54—N14	122.1 (3)
C15—C14—N2	122.2 (4)	C55—C54—N14	119.1 (3)
C16—C15—C14	119.6 (4)	C56—C55—C54	120.3 (3)
C16—C15—H15	120.2	C56—C55—H55	119.9
C14—C15—H15	120.2	C54—C55—H55	119.9
C17—C16—C15	121.2 (4)	C55—C56—C57	121.4 (4)
C17—C16—H16	119.4	C55—C56—H56	119.3
C15—C16—H16	119.4	C57—C56—H56	119.3
C18—C17—C16	119.4 (4)	C58—C57—C56	118.1 (4)

C18—C17—H17	120.3	C58—C57—H57	121.0
C16—C17—H17	120.3	C56—C57—H57	121.0
C17—C18—C19	121.1 (4)	C57—C58—C59	121.5 (3)
C17—C18—H18	119.5	C57—C58—H58	119.3
C19—C18—H18	119.5	C59—C58—H58	119.3
C14—C19—C18	119.8 (4)	C58—C59—C54	120.0 (3)
C14—C19—H19	120.1	C58—C59—H59	120.0
C18—C19—H19	120.1	C54—C59—H59	120.0
N3—C20—H20A	109.5	N15—C60—H60A	109.5
N3—C20—H20B	109.5	N15—C60—H60B	109.5
H20A—C20—H20B	109.5	H60A—C60—H60B	109.5
N3—C20—H20C	109.5	N15—C60—H60C	109.5
H20A—C20—H20C	109.5	H60A—C60—H60C	109.5
H20B—C20—H20C	109.5	H60B—C60—H60C	109.5
C21—S2—C22	90.80 (18)	C61—S4—C62	91.24 (18)
C21—N7—N8	113.0 (3)	C61—N19—N20	113.8 (3)
N7—N8—C34	116.0 (3)	N19—N20—C74	116.9 (3)
N7—N8—C22	117.9 (3)	N19—N20—C62	118.4 (3)
C34—N8—C22	124.2 (3)	C74—N20—C62	124.6 (3)
C23—N9—C22	124.5 (3)	C63—N21—C80	118.5 (4)
C23—N9—C40	118.8 (3)	C63—N21—C62	124.4 (3)
C22—N9—C40	116.7 (3)	C80—N21—C62	117.1 (3)
C23—N10—C24	111.0 (3)	C63—N22—C64	111.5 (3)
C26—N11—N12	105.1 (3)	C66—N23—N24	105.1 (4)
C24—N12—N11	110.9 (3)	N23—N24—C64	112.1 (3)
C24—N12—C27	128.2 (3)	N23—N24—C67	120.5 (4)
N11—N12—C27	120.8 (3)	C64—N24—C67	127.4 (4)
N7—C21—C28	122.6 (4)	N19—C61—C68	123.3 (4)
N7—C21—S2	115.5 (3)	N19—C61—S4	114.9 (3)
C28—C21—S2	121.9 (3)	C68—C61—S4	121.6 (3)
C25—C22—N9	107.5 (3)	N21—C62—N20	111.9 (3)
C25—C22—N8	114.5 (3)	N21—C62—C65	107.5 (3)
N9—C22—N8	111.9 (3)	N20—C62—C65	114.1 (3)
C25—C22—S2	111.2 (3)	N21—C62—S4	110.9 (3)
N9—C22—S2	110.9 (3)	N20—C62—S4	101.4 (2)
N8—C22—S2	100.8 (2)	C65—C62—S4	111.0 (3)
N10—C23—N9	127.7 (3)	N22—C63—N21	127.6 (4)
N10—C23—H23	116.1	N22—C63—H63	116.2
N9—C23—H23	116.1	N21—C63—H63	116.2
N12—C24—C25	107.6 (3)	N24—C64—N22	125.5 (4)
N12—C24—N10	124.4 (3)	N24—C64—C65	106.4 (4)
C25—C24—N10	128.0 (4)	N22—C64—C65	128.1 (4)
C24—C25—C26	104.5 (3)	C64—C65—C66	105.6 (4)
C24—C25—C22	121.3 (3)	C64—C65—C62	120.8 (4)
C26—C25—C22	134.2 (3)	C66—C65—C62	133.6 (3)
N11—C26—C25	111.8 (3)	N23—C66—C65	110.8 (3)
N11—C26—H26	124.1	N23—C66—H66	124.6
C25—C26—H26	124.1	C65—C66—H66	124.6

N12—C27—H27A	109.5	N24—C67—H67A	109.5
N12—C27—H27B	109.5	N24—C67—H67B	109.5
H27A—C27—H27B	109.5	H67A—C67—H67B	109.5
N12—C27—H27C	109.5	N24—C67—H67C	109.5
H27A—C27—H27C	109.5	H67A—C67—H67C	109.5
H27B—C27—H27C	109.5	H67B—C67—H67C	109.5
C29—C28—C33	118.5 (4)	C69—C68—C73	119.1 (4)
C29—C28—C21	121.0 (4)	C69—C68—C61	121.2 (4)
C33—C28—C21	120.5 (4)	C73—C68—C61	119.7 (4)
C30—C29—C28	121.7 (4)	C70—C69—C68	120.4 (4)
C30—C29—H29	119.2	C70—C69—H69	119.8
C28—C29—H29	119.2	C68—C69—H69	119.8
C29—C30—C31	119.3 (4)	C69—C70—C71	120.3 (5)
C29—C30—H30	120.3	C69—C70—H70	119.9
C31—C30—H30	120.3	C71—C70—H70	119.9
C32—C31—C30	119.9 (4)	C72—C71—C70	119.9 (4)
C32—C31—H31	120.0	C72—C71—H71	120.1
C30—C31—H31	120.0	C70—C71—H71	120.1
C31—C32—C33	120.3 (4)	C71—C72—C73	120.8 (4)
C31—C32—H32	119.9	C71—C72—H72	119.6
C33—C32—H32	119.9	C73—C72—H72	119.6
C32—C33—C28	120.3 (4)	C72—C73—C68	119.5 (4)
C32—C33—H33	119.9	C72—C73—H73	120.2
C28—C33—H33	119.9	C68—C73—H73	120.2
C39—C34—C35	119.0 (3)	C75—C74—C79	119.0 (4)
C39—C34—N8	122.5 (3)	C75—C74—N20	119.1 (4)
C35—C34—N8	118.5 (3)	C79—C74—N20	121.9 (4)
C36—C35—C34	120.2 (4)	C74—C75—C76	119.8 (4)
C36—C35—H35	119.9	C74—C75—H75	120.1
C34—C35—H35	119.9	C76—C75—H75	120.1
C35—C36—C37	121.5 (4)	C77—C76—C75	120.8 (4)
C35—C36—H36	119.2	C77—C76—H76	119.6
C37—C36—H36	119.2	C75—C76—H76	119.6
C38—C37—C36	117.9 (4)	C78—C77—C76	119.8 (4)
C38—C37—H37	121.0	C78—C77—H77	120.1
C36—C37—H37	121.0	C76—C77—H77	120.1
C37—C38—C39	121.6 (4)	C77—C78—C79	120.8 (4)
C37—C38—H38	119.2	C77—C78—H78	119.6
C39—C38—H38	119.2	C79—C78—H78	119.6
C34—C39—C38	119.7 (3)	C78—C79—C74	119.9 (4)
C34—C39—H39	120.2	C78—C79—H79	120.1
C38—C39—H39	120.2	C74—C79—H79	120.1
N9—C40—H40A	109.5	N21—C80—H80A	109.5
N9—C40—H40B	109.5	N21—C80—H80B	109.5
H40A—C40—H40B	109.5	H80A—C80—H80B	109.5
N9—C40—H40C	109.5	N21—C80—H80C	109.5
H40A—C40—H40C	109.5	H80A—C80—H80C	109.5
H40B—C40—H40C	109.5	H80B—C80—H80C	109.5

C1—N1—N2—C14	177.6 (4)	C41—N13—N14—C54	−175.9 (4)
C1—N1—N2—C2	9.3 (5)	C41—N13—N14—C42	6.4 (6)
C6—N5—N6—C4	−0.1 (5)	C46—N17—N18—C44	−0.1 (5)
C6—N5—N6—C7	179.7 (4)	C46—N17—N18—C47	178.2 (4)
N2—N1—C1—C8	177.9 (4)	N14—N13—C41—C48	177.7 (4)
N2—N1—C1—S1	0.6 (5)	N14—N13—C41—S3	−0.9 (5)
C2—S1—C1—N1	−7.3 (4)	C42—S3—C41—N13	−3.3 (4)
C2—S1—C1—C8	175.4 (4)	C42—S3—C41—C48	178.0 (4)
C3—N3—C2—N2	124.3 (4)	C43—N15—C42—C45	−0.4 (5)
C20—N3—C2—N2	−54.3 (5)	C60—N15—C42—C45	179.3 (4)
C3—N3—C2—C5	−2.6 (5)	C43—N15—C42—N14	126.1 (4)
C20—N3—C2—C5	178.7 (4)	C60—N15—C42—N14	−54.2 (5)
C3—N3—C2—S1	−123.3 (4)	C43—N15—C42—S3	−122.0 (4)
C20—N3—C2—S1	58.1 (4)	C60—N15—C42—S3	57.6 (4)
N1—N2—C2—N3	105.1 (4)	N13—N14—C42—C45	−127.6 (4)
C14—N2—C2—N3	−62.2 (5)	C54—N14—C42—C45	54.9 (5)
N1—N2—C2—C5	−131.8 (4)	N13—N14—C42—N15	109.8 (4)
C14—N2—C2—C5	60.9 (5)	C54—N14—C42—N15	−67.7 (5)
N1—N2—C2—S1	−13.3 (4)	N13—N14—C42—S3	−8.0 (4)
C14—N2—C2—S1	179.4 (3)	C54—N14—C42—S3	174.5 (3)
C1—S1—C2—N3	−108.9 (3)	C41—S3—C42—C45	127.6 (3)
C1—S1—C2—N2	10.6 (3)	C41—S3—C42—N15	−112.9 (3)
C1—S1—C2—C5	132.1 (3)	C41—S3—C42—N14	5.7 (3)
C4—N4—C3—N3	1.2 (6)	C44—N16—C43—N15	0.4 (6)
C20—N3—C3—N4	179.1 (4)	C42—N15—C43—N16	0.0 (7)
C2—N3—C3—N4	0.5 (7)	C60—N15—C43—N16	−179.6 (4)
N5—N6—C4—N4	−177.8 (4)	N17—N18—C44—N16	−179.4 (4)
C7—N6—C4—N4	2.4 (7)	C47—N18—C44—N16	2.4 (7)
N5—N6—C4—C5	1.1 (5)	N17—N18—C44—C45	0.7 (5)
C7—N6—C4—C5	−178.7 (5)	C47—N18—C44—C45	−177.4 (4)
C3—N4—C4—N6	178.3 (4)	C43—N16—C44—N18	179.9 (4)
C3—N4—C4—C5	−0.4 (6)	C43—N16—C44—C45	−0.3 (6)
N6—C4—C5—C6	−1.6 (5)	N18—C44—C45—C46	−1.1 (4)
N4—C4—C5—C6	177.3 (4)	N16—C44—C45—C46	179.1 (4)
N6—C4—C5—C2	179.1 (4)	N18—C44—C45—C42	179.8 (3)
N4—C4—C5—C2	−2.0 (7)	N16—C44—C45—C42	−0.1 (6)
N3—C2—C5—C4	3.2 (5)	N15—C42—C45—C44	0.4 (5)
N2—C2—C5—C4	−122.5 (4)	N14—C42—C45—C44	−124.5 (4)
S1—C2—C5—C4	124.3 (4)	S3—C42—C45—C44	121.7 (4)
N3—C2—C5—C6	−175.9 (4)	N15—C42—C45—C46	−178.5 (4)
N2—C2—C5—C6	58.4 (6)	N14—C42—C45—C46	56.5 (6)
S1—C2—C5—C6	−54.8 (5)	S3—C42—C45—C46	−57.2 (5)
N6—N5—C6—C5	−0.9 (5)	N18—N17—C46—C45	−0.6 (5)
C4—C5—C6—N5	1.6 (5)	C44—C45—C46—N17	1.1 (5)
C2—C5—C6—N5	−179.2 (4)	C42—C45—C46—N17	−179.9 (4)
N1—C1—C8—C13	164.7 (4)	N13—C41—C48—C53	−13.7 (7)
S1—C1—C8—C13	−18.2 (6)	S3—C41—C48—C53	164.8 (4)

N1—C1—C8—C9	−15.6 (7)	N13—C41—C48—C49	168.3 (5)
S1—C1—C8—C9	161.4 (3)	S3—C41—C48—C49	−13.2 (6)
C13—C8—C9—C10	−0.3 (7)	C53—C48—C49—C50	0.5 (8)
C1—C8—C9—C10	−180.0 (4)	C41—C48—C49—C50	178.6 (5)
C8—C9—C10—C11	0.2 (8)	C48—C49—C50—C51	−0.3 (8)
C9—C10—C11—C12	0.4 (8)	C49—C50—C51—C52	0.3 (8)
C10—C11—C12—C13	−0.8 (9)	C50—C51—C52—C53	−0.5 (8)
C11—C12—C13—C8	0.6 (9)	C51—C52—C53—C48	0.8 (8)
C9—C8—C13—C12	−0.1 (8)	C49—C48—C53—C52	−0.8 (8)
C1—C8—C13—C12	179.6 (5)	C41—C48—C53—C52	−178.8 (5)
N1—N2—C14—C19	16.9 (5)	N13—N14—C54—C59	−164.1 (4)
C2—N2—C14—C19	−175.6 (4)	C42—N14—C54—C59	13.4 (6)
N1—N2—C14—C15	−163.7 (4)	N13—N14—C54—C55	15.5 (6)
C2—N2—C14—C15	3.7 (6)	C42—N14—C54—C55	−167.0 (4)
C19—C14—C15—C16	−0.7 (6)	C59—C54—C55—C56	0.4 (6)
N2—C14—C15—C16	179.9 (4)	N14—C54—C55—C56	−179.1 (4)
C14—C15—C16—C17	0.5 (6)	C54—C55—C56—C57	−0.1 (7)
C15—C16—C17—C18	0.1 (7)	C55—C56—C57—C58	0.1 (7)
C16—C17—C18—C19	−0.3 (8)	C56—C57—C58—C59	−0.4 (6)
C15—C14—C19—C18	0.5 (6)	C57—C58—C59—C54	0.8 (6)
N2—C14—C19—C18	179.9 (4)	C55—C54—C59—C58	−0.8 (6)
C17—C18—C19—C14	0.0 (7)	N14—C54—C59—C58	178.8 (4)
C21—N7—N8—C34	−176.4 (4)	C61—N19—N20—C74	175.5 (4)
C21—N7—N8—C22	−11.6 (5)	C61—N19—N20—C62	−2.3 (6)
C26—N11—N12—C24	−0.1 (4)	C66—N23—N24—C64	0.3 (5)
C26—N11—N12—C27	−178.7 (4)	C66—N23—N24—C67	−178.7 (4)
N8—N7—C21—C28	−177.9 (4)	N20—N19—C61—C68	−177.8 (4)
N8—N7—C21—S2	1.2 (5)	N20—N19—C61—S4	−1.5 (5)
C22—S2—C21—N7	6.5 (4)	C62—S4—C61—N19	3.6 (4)
C22—S2—C21—C28	−174.3 (4)	C62—S4—C61—C68	179.9 (4)
C23—N9—C22—C25	2.4 (5)	C63—N21—C62—N20	−123.6 (4)
C40—N9—C22—C25	−179.0 (3)	C80—N21—C62—N20	55.6 (5)
C23—N9—C22—N8	−124.2 (4)	C63—N21—C62—C65	2.4 (5)
C40—N9—C22—N8	54.4 (5)	C80—N21—C62—C65	−178.4 (4)
C23—N9—C22—S2	124.1 (4)	C63—N21—C62—S4	124.0 (4)
C40—N9—C22—S2	−57.3 (4)	C80—N21—C62—S4	−56.8 (4)
N7—N8—C22—C25	134.3 (4)	N19—N20—C62—N21	−113.7 (4)
C34—N8—C22—C25	−62.3 (5)	C74—N20—C62—N21	68.6 (5)
N7—N8—C22—N9	−103.1 (4)	N19—N20—C62—C65	123.9 (4)
C34—N8—C22—N9	60.3 (5)	C74—N20—C62—C65	−53.7 (5)
N7—N8—C22—S2	14.8 (4)	N19—N20—C62—S4	4.5 (4)
C34—N8—C22—S2	178.2 (3)	C74—N20—C62—S4	−173.1 (3)
C21—S2—C22—C25	−132.7 (3)	C61—S4—C62—N21	114.8 (3)
C21—S2—C22—N9	107.7 (3)	C61—S4—C62—N20	−4.1 (3)
C21—S2—C22—N8	−10.9 (3)	C61—S4—C62—C65	−125.7 (3)
C24—N10—C23—N9	−1.7 (6)	C64—N22—C63—N21	−0.9 (6)
C22—N9—C23—N10	−0.2 (6)	C80—N21—C63—N22	−179.9 (4)
C40—N9—C23—N10	−178.8 (4)	C62—N21—C63—N22	−0.7 (7)

N11—N12—C24—C25	−0.7 (4)	N23—N24—C64—N22	178.7 (4)
C27—N12—C24—C25	177.7 (4)	C67—N24—C64—N22	−2.4 (8)
N11—N12—C24—N10	178.8 (4)	N23—N24—C64—C65	−1.1 (5)
C27—N12—C24—N10	−2.7 (7)	C67—N24—C64—C65	177.8 (5)
C23—N10—C24—N12	−178.2 (4)	C63—N22—C64—N24	−179.2 (4)
C23—N10—C24—C25	1.2 (6)	C63—N22—C64—C65	0.6 (6)
N12—C24—C25—C26	1.2 (4)	N24—C64—C65—C66	1.4 (5)
N10—C24—C25—C26	−178.3 (4)	N22—C64—C65—C66	−178.3 (4)
N12—C24—C25—C22	−179.4 (3)	N24—C64—C65—C62	−178.8 (4)
N10—C24—C25—C22	1.1 (6)	N22—C64—C65—C62	1.4 (7)
N9—C22—C25—C24	−2.7 (5)	N21—C62—C65—C64	−2.7 (5)
N8—C22—C25—C24	122.3 (4)	N20—C62—C65—C64	122.0 (4)
S2—C22—C25—C24	−124.2 (3)	S4—C62—C65—C64	−124.2 (4)
N9—C22—C25—C26	176.5 (4)	N21—C62—C65—C66	177.0 (4)
N8—C22—C25—C26	−58.4 (6)	N20—C62—C65—C66	−58.3 (6)
S2—C22—C25—C26	55.0 (5)	S4—C62—C65—C66	55.5 (6)
N12—N11—C26—C25	0.9 (5)	N24—N23—C66—C65	0.6 (5)
C24—C25—C26—N11	−1.3 (5)	C64—C65—C66—N23	−1.3 (5)
C22—C25—C26—N11	179.3 (4)	C62—C65—C66—N23	178.9 (4)
N7—C21—C28—C29	18.0 (7)	N19—C61—C68—C69	−169.2 (4)
S2—C21—C28—C29	−161.1 (4)	S4—C61—C68—C69	14.8 (6)
N7—C21—C28—C33	−162.6 (4)	N19—C61—C68—C73	12.0 (7)
S2—C21—C28—C33	18.3 (6)	S4—C61—C68—C73	−164.0 (3)
C33—C28—C29—C30	0.6 (7)	C73—C68—C69—C70	−0.1 (8)
C21—C28—C29—C30	180.0 (4)	C61—C68—C69—C70	−179.0 (5)
C28—C29—C30—C31	−0.6 (8)	C68—C69—C70—C71	−0.8 (9)
C29—C30—C31—C32	0.3 (8)	C69—C70—C71—C72	1.2 (9)
C30—C31—C32—C33	0.1 (8)	C70—C71—C72—C73	−0.7 (8)
C31—C32—C33—C28	−0.1 (8)	C71—C72—C73—C68	−0.3 (8)
C29—C28—C33—C32	−0.2 (7)	C69—C68—C73—C72	0.6 (7)
C21—C28—C33—C32	−179.6 (5)	C61—C68—C73—C72	179.5 (5)
N7—N8—C34—C39	160.5 (4)	N19—N20—C74—C75	−14.6 (6)
C22—N8—C34—C39	−3.1 (6)	C62—N20—C74—C75	163.0 (4)
N7—N8—C34—C35	−19.9 (5)	N19—N20—C74—C79	164.4 (4)
C22—N8—C34—C35	176.4 (4)	C62—N20—C74—C79	−17.9 (6)
C39—C34—C35—C36	−0.6 (6)	C79—C74—C75—C76	−0.8 (7)
N8—C34—C35—C36	179.8 (4)	N20—C74—C75—C76	178.3 (4)
C34—C35—C36—C37	−0.3 (7)	C74—C75—C76—C77	−0.3 (7)
C35—C36—C37—C38	0.8 (7)	C75—C76—C77—C78	0.5 (8)
C36—C37—C38—C39	−0.4 (7)	C76—C77—C78—C79	0.3 (7)
C35—C34—C39—C38	1.0 (6)	C77—C78—C79—C74	−1.3 (6)
N8—C34—C39—C38	−179.5 (3)	C75—C74—C79—C78	1.6 (6)
C37—C38—C39—C34	−0.5 (6)	N20—C74—C79—C78	−177.5 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···N11^{i}	0.95	2.49	3.247 (5)	137

C7—H7*C*···N22	0.98	2.49	3.382 (6)	151
C23—H23···N5	0.95	2.41	3.232 (5)	144
C43—H43···N23^{ii}	0.95	2.60	3.286 (5)	129
C59—H59···N15	0.95	2.56	3.144 (5)	120
C63—H63···N17	0.95	2.53	3.284 (5)	137
C67—H67*C*···N4	0.98	2.57	3.472 (6)	153
C79—H79···N21	0.95	2.54	3.140 (5)	121

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