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Crystal structure of (*E*)-1-(3-benzyl-5-phenyl-1,3-thiazol-2-ylidene)-2-[(*E*)-1,2,3,4-tetrahydronaphthalen-1-ylidene]hydrazin-1-ium bromide

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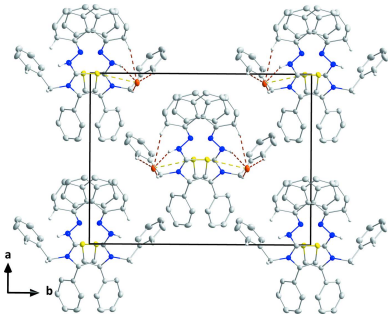
In the title molecular salt, $C_{26}H_{24}N_3S^+\cdot Br^-$, the dihedral angles between the thiazole ring and its attached phenyl and benzoyl rings are 54.81 (7) and 85.51 (7)°, respectively. In the crystal, ion pairs are linked by C—H···Br and N—H···Br hydrogen bonds and are connected into helical chains extending along the *c*-axis direction by weak, electrostatic S···Br^- interactions. A Hirshfeld surface analysis was performed, which showed the dominant role of H···H contacts (51.3%).

1. Chemical context

Thiazoles are a class of heterocyclic compounds found in many biologically active drugs such as sulfathiazol (antimicrobial drug), ritonavir (antiretroviral drug), abafungin (antifungal drug) and tiazofurin (antineoplastic drug) (Siddiqui *et al.*, 2009). Other compounds containing the thiazole or thiazolyl moiety show numerous biological activities such as antimicrobial and antifungal (Vasu *et al.*, 2013), anti-inflammatory (Singh *et al.*, 2008), anticancer (Luzina *et al.*, 2009), antihypertensive (Turan-Zitouni *et al.*, 2000), anti-HIV (Rawal *et al.*, 2008), anticonvulsant (Satoh *et al.*, 2009) and antidiabetic properties (Iino *et al.*, 2009). As with many biologically active molecules, the molecular conformation adopted may have a significant effect on the activity which prompted an examination of the crystal structure of the title salt, $C_{26}H_{24}N_3S\cdot Br$, **I** (Fig. 1).



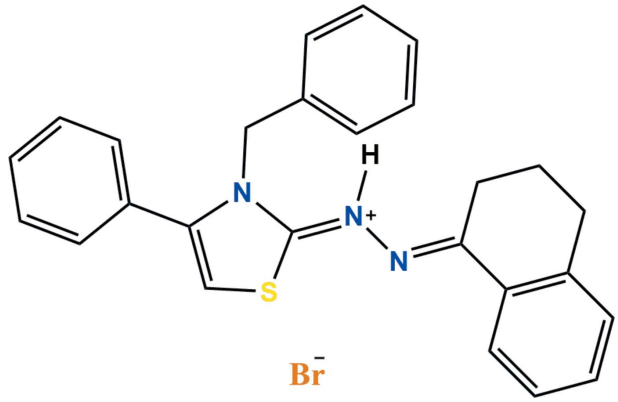


Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···Br1^{i}	0.91	2.63	3.4633 (18)	152
C10—H10B···Br1^{i}	0.99	2.88	3.837 (2)	164
C20—H20B···Br1^{i}	0.99	2.84	3.7560 (19)	155
C26—H26···Br1^{i}	0.95	2.90	3.730 (2)	146

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

2. Structural commentary

As expected, the C11/C12/C13/N3/S1 thiazole ring in **I** is almost planar (r.m.s. deviation = 0.0056 Å) and the mean planes of the C14–C19 and C21–C26 benzene rings are inclined to this plane by 54.81 (7) and 85.51 (7)°, respectively. The dihedral angle between the mean planes of the thiazole and C2–C7 rings is 13.1 (1)°. A puckering analysis of the C1/C2/C7–C10 ring yielded the parameters Q = 0.499 (3) Å, θ = 58.6 (3)° and φ = 225.6 (3)°, indicating a half-chair conformation.

3. Supramolecular features

In the crystal, the S1···Br1 distance of 3.5017 (7) Å is some 0.15 Å less than the sum of the van der Waals radii and likely represents an electrostatic interaction between the two atoms since S1 is near to the cationic charge. Over 200 structures having S···Br^{-} contacts of this length or shorter are present in the Cambridge Structural Database, two examples being reported by Auffinger *et al.* (2004) and Thompson & Richardson (1977). This interaction, together with the N2—H2···Br1, C10—H10B···Br1, C20—H20B···Br1 and C26—H26···Br1 hydrogen bonds (Table 1) form helical chains extending along the *c*-axis direction (Fig. 2). It may be noted that the same bromide ion Br1(x, 1 − y, $z-\frac{1}{2}$) accepts all the identified contacts. These [001] chains pack in the other two dimensions with normal van der Waals contacts (Fig. 3), in agreement with the results of the Hirshfeld surface analysis (*vide infra*).

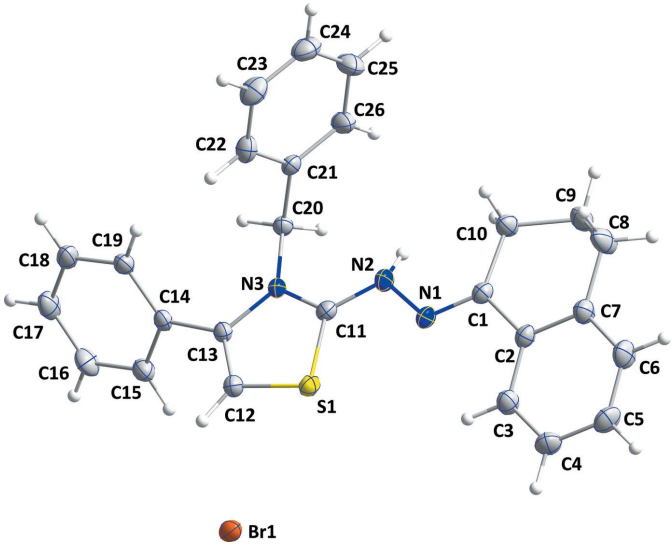


Figure 1
The title molecule showing 50% probability ellipsoids.

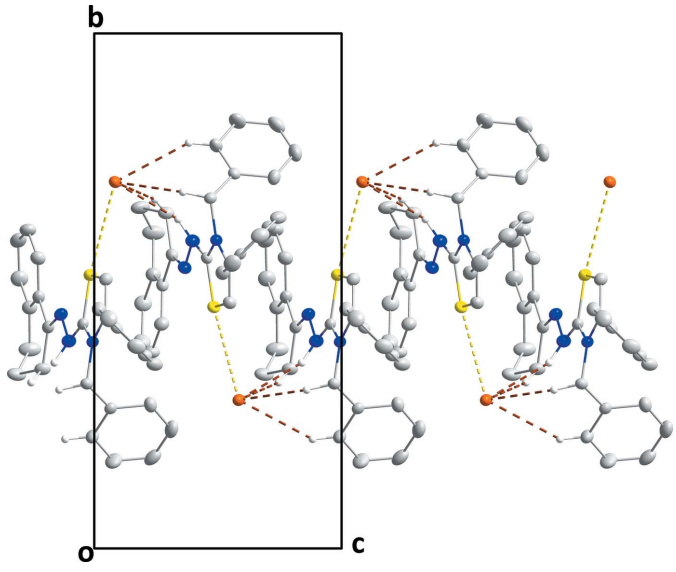


Figure 2
Detail of a supramolecular chain viewed along the *a*-axis direction with C—H···Br and N—H···Br hydrogen bonds depicted by brown dashed lines. The short Br···S contact is depicted by a yellow dashed line.

4. Database survey

A search of the Cambridge Structural Database (CSD, updated to Dec. 31, 2020; Groom, *et al.*, 2016) using the fragment **A** yielded 30 hits of which 11 were considered similar to **I**. Among these, (*Z*)-1-[(2*E*)-3,4-diphenyl-2,3-dihydro-1,3-thiazol-2-ylidene]-2-[1-(4-hydroxyphenyl)ethylidene]hydra-

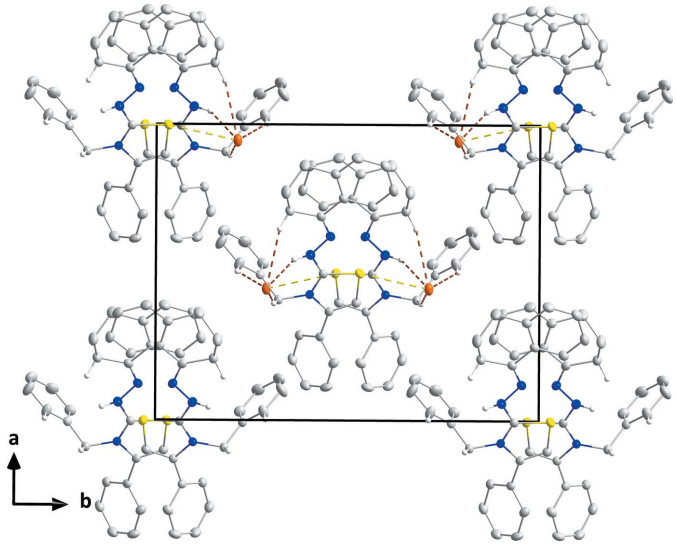
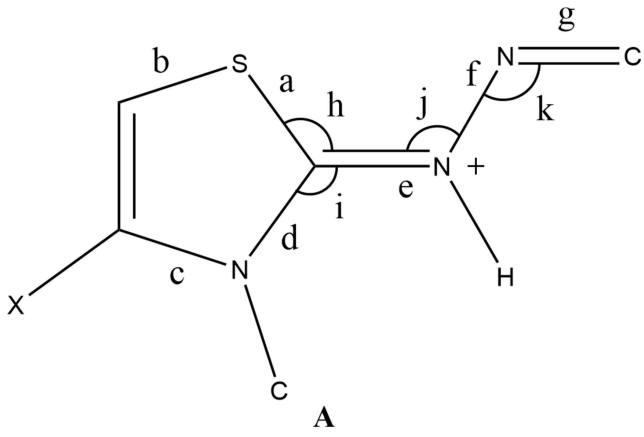


Figure 3
Packing seen along the *c*-axis direction giving an end view of the chains. Intermolecular interactions are depicted as in Fig. 2.

zinium bromide unknown solvate (CSD refcode BOCROC; Mague, *et al.*, 2014) and (*E*)-2-[(2-nitrophenyl)methylidene]-1-[(2*Z*)-4-phenyl-2,3-dihydro-1,3-thiazol-2-ylidene]hydrazinium bromide (NUCLOO; Hassan *et al.*, 2016) are the closest analogues and another similar compound is 2-{1-[(3,4-diphenyl-1,3-thiazol-2(3*H*)-ylidene)hydrazinylidene]ethyl}-pyridinium bromide monohydrate (QOCGIA; Akkurt *et al.*, 2014). Key bond distances and angles for **I** and these three compounds are listed in supplementary Table 1. In the thiazole ring there is little variation except for the N—C distance *c* in NUCLOO, which is marginally shorter than in the others, possibly due to the nitrogen atom being unsubstituted. The most noticeable differences occur in the N—C and C═N distances *d* and *e* where the difference between the two is largest in QOCGIA where the absence of the positive charge on the nitrogen atom bound to the thiazole ring leads to a greater localization of the π-electron density in the C═N bond.



A

5. Hirshfeld surface analysis

The Hirshfeld surface for **I** was calculated using *Crystal Explorer17* (Turner *et al.*, 2017) following the procedures described by Tan *et al.* (2019). Fig. 4*a* presents the Hirshfeld surface plotted over d_{norm} with a second cation closest to the bromide ion also present, clearly showing the N—H···Br and C—H···Br interactions as well as the S1···Br1 short contact (dashed lines). The surface plotted over shape (Fig. 4*b*) and curvature indices (Fig. 4*c*) do not show much flat surface or evidence for π-stacking interactions, in agreement with the results given in Section 3. Fig. 5 presents fingerprint plots for all intermolecular interactions (*a*) and resolved into all H···H contacts (*b*, 51.3%), H···C/C···H contacts (*c*, 21.9%), Br···H/H···Br contacts (*d*, 14.1%) and S···H/H···S contacts (*d*, 3.3%). The N···H/H···N contacts contribute only 1.3%.

6. Synthesis and crystallization

The title compound was prepared according to our previously reported method (Mohamed *et al.*, 2013). Mono-crystals of **I** suitable for X-ray diffraction were obtained by recrystallization of the crude product from ethanol solution.

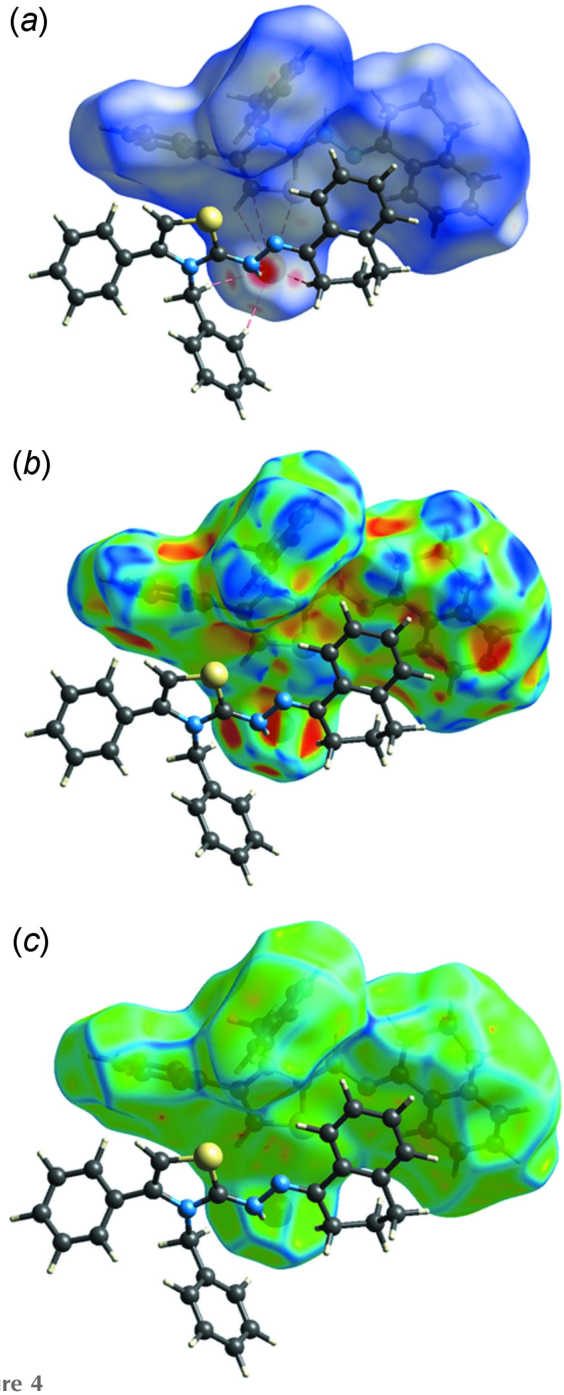


Figure 4
The Hirshfeld surface plotted over (*a*) d_{norm} and (*b*) shape and (*c*) curvature indices.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms attached to carbon were placed in calculated positions (C—H = 0.95–0.99 Å) while that attached to nitrogen was placed in a location derived from a difference map and its coordinates adjusted to give N—H = 0.91 Å. All were included as riding contributions with isotropic displacement parameters 1.2–1.5 times those of the attached atoms.

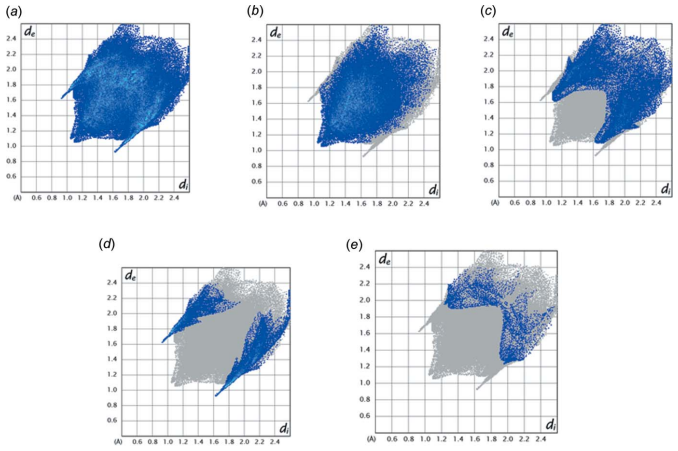


Figure 5
Fingerprint plots showing all (*a*) interactions and resolved into (*b*) H···H, (*c*) H···C/C···H, (*d*) Br···H/H···Br and (*e*) S···H/H···S contacts.

Funding information

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Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{26}H_{24}N_3S^+\cdot Br^-$
M_r	490.45
Crystal system, space group	Monoclinic, *Cc*
Temperature (K)	150
a, *b*, *c* (Å)	14.5474 (7), 17.8777 (8), 9.0803 (4)
β (°)	108.773 (2)
V (Å^3)	2235.92 (18)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.95
Crystal size (mm)	0.22 × 0.12 × 0.06
Data collection	
Diffractometer	Bruker D8 QUEST PHOTON 3 diffractometer
Absorption correction	Numerical (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.69, 0.89
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	48057, 6797, 6460
R_{int}	0.026
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.715
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.023, 0.052, 1.03
No. of reflections	6797
No. of parameters	280
No. of restraints	2
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.56, −0.22
Absolute structure	Parsons *et al.* (2013)
Absolute structure parameter	0.0130 (18)

Computer programs: *APEX3* and *SAINT* (Bruker, 2020), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018/1* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

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supporting information

Acta Cryst. (2021). E**77**, 420-423 [https://doi.org/10.1107/S2056989021002863]

Crystal structure of (*E*)-1-(3-benzyl-5-phenyl-1,3-thiazol-2-yl-idene)-2-[(*E*)-1,2,3,4-tetrahydronaphthalen-1-ylidene]hydrazin-1-ium bromide

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Computing details

Data collection: *APEX3* (Bruker, 2020); cell refinement: *SAINT* (Bruker, 2020); data reduction: *SAINT* (Bruker, 2020); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015*a*); program(s) used to refine structure: *SHELXL2018/1* (Sheldrick, 2015*b*); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2012); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

(*E*)-1-(3-Benzyl-5-phenyl-1,3-thiazol-2-ylidene)-2-[(*E*)-1,2,3,4-tetrahydronaphthalen-1-ylidene]hydrazin-1-ium bromide

Crystal data

$C_{26}H_{24}N_3S^+\cdot Br^-$
M_r = 490.45
Monoclinic, *Cc*
a = 14.5474 (7) Å
b = 17.8777 (8) Å
c = 9.0803 (4) Å
β = 108.773 (2)°
V = 2235.92 (18) Å^3
Z = 4
F(000) = 1008
D_x = 1.457 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 9847 reflections
θ = 2.6–30.5°
μ = 1.95 mm^{-1}
T = 150 K
Column, colourless
0.22 × 0.12 × 0.06 mm

Data collection

Bruker D8 QUEST PHOTON 3 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 7.3910 pixels mm^{-1}
φ and *ω* scans
Absorption correction: numerical (*SADABS*; Krause *et al.*, 2015)
T_{min} = 0.69, T_{max} = 0.89
48057 measured reflections
6797 independent reflections
6460 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 30.6°, θ_{min} = 2.6°
h = −20→20
k = −25→25
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.052
S = 1.03
6797 reflections
280 parameters
2 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0262P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.56$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}
Absolute structure: Parsons *et al.* (2013)
Absolute structure parameter: 0.0130 (18)

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger. H-atoms attached to carbon were placed in calculated positions (C—H = 0.95 - 0.99 Å) while that attached to nitrogen was placed in a location derived from a difference map and its coordinates adjusted to give N—H = 0.91 %A. All were included as riding contributions with isotropic displacement parameters 1.2 - 1.5 times those of the attached atoms.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.44542 (2)	0.28839 (2)	0.58421 (2)	0.02486 (6)
S1	0.49752 (4)	0.46885 (3)	0.48367 (6)	0.02090 (10)
N1	0.62223 (12)	0.54541 (10)	0.3655 (2)	0.0209 (3)
N2	0.55946 (13)	0.59721 (10)	0.3976 (2)	0.0224 (4)
H2	0.543925	0.639353	0.338574	0.027*
N3	0.42532 (11)	0.59882 (9)	0.49354 (19)	0.0175 (3)
C1	0.68896 (14)	0.57005 (11)	0.3140 (2)	0.0200 (4)
C2	0.74987 (14)	0.51162 (12)	0.2755 (2)	0.0204 (4)
C3	0.72405 (16)	0.43611 (12)	0.2725 (3)	0.0253 (4)
H3	0.668268	0.422211	0.298899	0.030*
C4	0.77838 (18)	0.38168 (12)	0.2319 (3)	0.0292 (5)
H4	0.760010	0.330612	0.230188	0.035*
C5	0.86007 (17)	0.40157 (14)	0.1934 (3)	0.0307 (5)
H5	0.897430	0.364250	0.164362	0.037*
C6	0.88672 (17)	0.47585 (13)	0.1977 (3)	0.0307 (5)
H6	0.943027	0.489020	0.172126	0.037*
C7	0.83287 (15)	0.53211 (12)	0.2386 (3)	0.0247 (4)
C8	0.86140 (18)	0.61314 (13)	0.2398 (4)	0.0377 (6)
H8A	0.900626	0.620413	0.169772	0.045*
H8B	0.901484	0.627820	0.346198	0.045*
C9	0.77120 (19)	0.66194 (13)	0.1863 (3)	0.0335 (5)
H9A	0.732936	0.648836	0.077981	0.040*
H9B	0.790648	0.715091	0.188104	0.040*
C10	0.70864 (16)	0.65141 (12)	0.2911 (3)	0.0251 (4)
H10A	0.741830	0.674405	0.393677	0.030*
H10B	0.646075	0.677709	0.244715	0.030*
C11	0.49537 (14)	0.56397 (11)	0.4544 (2)	0.0181 (4)
C12	0.39810 (15)	0.47730 (11)	0.5475 (2)	0.0212 (4)

H12	0.368071	0.436044	0.579688	0.025*
C13	0.36779 (14)	0.54826 (10)	0.5468 (2)	0.0174 (4)
C14	0.28248 (14)	0.57165 (11)	0.5907 (2)	0.0181 (4)
C15	0.19406 (15)	0.53523 (12)	0.5184 (2)	0.0248 (4)
H15	0.189962	0.497890	0.442080	0.030*
C16	0.11274 (16)	0.55376 (13)	0.5583 (3)	0.0313 (5)
H16	0.052661	0.529488	0.508398	0.038*
C17	0.11875 (17)	0.60770 (13)	0.6709 (3)	0.0307 (5)
H17	0.062685	0.620568	0.697431	0.037*
C18	0.20603 (17)	0.64264 (12)	0.7444 (3)	0.0273 (5)
H18	0.210020	0.678992	0.822524	0.033*
C19	0.28772 (16)	0.62514 (11)	0.7051 (3)	0.0214 (4)
H19	0.347538	0.649539	0.756080	0.026*
C20	0.40757 (14)	0.68028 (11)	0.4697 (2)	0.0189 (4)
H20A	0.348715	0.693577	0.496169	0.023*
H20B	0.394775	0.692002	0.358296	0.023*
C21	0.49177 (14)	0.72801 (11)	0.5665 (2)	0.0188 (4)
C22	0.52950 (17)	0.72086 (12)	0.7273 (3)	0.0261 (4)
H22	0.505130	0.683350	0.778964	0.031*
C23	0.60270 (18)	0.76845 (15)	0.8124 (3)	0.0329 (5)
H23	0.627952	0.763814	0.922321	0.039*
C24	0.63909 (17)	0.82285 (15)	0.7369 (3)	0.0345 (5)
H24	0.689705	0.855074	0.795090	0.041*
C25	0.60187 (18)	0.82998 (14)	0.5785 (3)	0.0371 (6)
H25	0.626501	0.867479	0.527208	0.044*
C26	0.52811 (19)	0.78259 (12)	0.4922 (3)	0.0287 (5)
H26	0.502782	0.787744	0.382335	0.034*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.03693 (11)	0.01870 (9)	0.02011 (9)	0.00145 (9)	0.01078 (7)	0.00129 (8)
S1	0.0231 (2)	0.0190 (2)	0.0225 (2)	0.00341 (19)	0.01004 (18)	−0.00098 (19)
N1	0.0207 (8)	0.0209 (8)	0.0239 (8)	0.0026 (7)	0.0109 (7)	−0.0022 (7)
N2	0.0229 (8)	0.0213 (9)	0.0274 (9)	0.0018 (7)	0.0144 (7)	−0.0006 (7)
N3	0.0185 (8)	0.0170 (7)	0.0193 (8)	−0.0005 (6)	0.0091 (6)	−0.0005 (6)
C1	0.0196 (9)	0.0208 (9)	0.0195 (9)	0.0018 (8)	0.0061 (7)	−0.0012 (7)
C2	0.0201 (9)	0.0220 (10)	0.0201 (9)	0.0036 (8)	0.0077 (8)	−0.0008 (8)
C3	0.0248 (10)	0.0241 (10)	0.0297 (11)	0.0029 (8)	0.0123 (9)	0.0023 (8)
C4	0.0337 (12)	0.0202 (10)	0.0356 (12)	0.0037 (9)	0.0139 (10)	−0.0005 (9)
C5	0.0297 (12)	0.0287 (11)	0.0356 (12)	0.0090 (9)	0.0130 (10)	−0.0043 (9)
C6	0.0247 (11)	0.0332 (12)	0.0400 (13)	0.0041 (9)	0.0182 (10)	−0.0003 (10)
C7	0.0222 (10)	0.0250 (10)	0.0297 (11)	0.0013 (8)	0.0122 (9)	−0.0002 (9)
C8	0.0313 (13)	0.0271 (12)	0.0657 (18)	−0.0026 (9)	0.0310 (13)	−0.0010 (12)
C9	0.0422 (13)	0.0214 (10)	0.0471 (15)	−0.0008 (10)	0.0288 (12)	0.0040 (10)
C10	0.0252 (11)	0.0198 (10)	0.0342 (12)	0.0015 (8)	0.0149 (9)	−0.0004 (9)
C11	0.0194 (9)	0.0179 (9)	0.0169 (9)	0.0003 (7)	0.0058 (7)	−0.0019 (7)
C12	0.0217 (9)	0.0209 (9)	0.0234 (10)	−0.0016 (8)	0.0105 (8)	−0.0014 (8)

C13	0.0187 (9)	0.0180 (9)	0.0165 (8)	−0.0007 (7)	0.0069 (7)	0.0012 (7)
C14	0.0187 (9)	0.0174 (9)	0.0199 (9)	0.0005 (7)	0.0086 (7)	0.0039 (7)
C15	0.0245 (10)	0.0258 (11)	0.0250 (10)	−0.0049 (8)	0.0094 (8)	−0.0002 (8)
C16	0.0195 (10)	0.0370 (13)	0.0385 (13)	−0.0060 (9)	0.0109 (9)	0.0022 (10)
C17	0.0252 (11)	0.0296 (12)	0.0441 (13)	0.0042 (9)	0.0205 (10)	0.0047 (10)
C18	0.0336 (12)	0.0206 (10)	0.0350 (12)	0.0037 (9)	0.0213 (10)	0.0013 (9)
C19	0.0229 (10)	0.0180 (9)	0.0255 (10)	−0.0007 (8)	0.0110 (8)	0.0014 (8)
C20	0.0209 (9)	0.0167 (9)	0.0209 (9)	0.0008 (7)	0.0092 (8)	0.0008 (7)
C21	0.0203 (10)	0.0177 (9)	0.0203 (9)	0.0013 (7)	0.0094 (8)	−0.0022 (7)
C22	0.0273 (11)	0.0310 (11)	0.0213 (10)	0.0025 (8)	0.0096 (9)	0.0025 (8)
C23	0.0305 (12)	0.0409 (13)	0.0233 (11)	0.0029 (10)	0.0031 (9)	−0.0048 (10)
C24	0.0307 (12)	0.0338 (13)	0.0373 (13)	−0.0052 (10)	0.0088 (10)	−0.0148 (10)
C25	0.0446 (15)	0.0309 (13)	0.0370 (13)	−0.0187 (11)	0.0151 (11)	−0.0066 (10)
C26	0.0398 (13)	0.0245 (11)	0.0225 (11)	−0.0089 (9)	0.0110 (10)	−0.0032 (8)

Geometric parameters (Å, º)

S1—C11	1.720 (2)	C10—H10B	0.9900
S1—C12	1.729 (2)	C12—C13	1.342 (3)
N1—C1	1.283 (3)	C12—H12	0.9500
N1—N2	1.396 (2)	C13—C14	1.480 (3)
N2—C11	1.341 (3)	C14—C19	1.396 (3)
N2—H2	0.9100	C14—C15	1.402 (3)
N3—C11	1.337 (2)	C15—C16	1.384 (3)
N3—C13	1.419 (2)	C15—H15	0.9500
N3—C20	1.483 (2)	C16—C17	1.388 (3)
C1—C2	1.483 (3)	C16—H16	0.9500
C1—C10	1.510 (3)	C17—C18	1.379 (3)
C2—C3	1.399 (3)	C17—H17	0.9500
C2—C7	1.402 (3)	C18—C19	1.382 (3)
C3—C4	1.377 (3)	C18—H18	0.9500
C3—H3	0.9500	C19—H19	0.9500
C4—C5	1.388 (3)	C20—C21	1.519 (3)
C4—H4	0.9500	C20—H20A	0.9900
C5—C6	1.381 (3)	C20—H20B	0.9900
C5—H5	0.9500	C21—C26	1.384 (3)
C6—C7	1.397 (3)	C21—C22	1.391 (3)
C6—H6	0.9500	C22—C23	1.387 (3)
C7—C8	1.506 (3)	C22—H22	0.9500
C8—C9	1.519 (4)	C23—C24	1.389 (4)
C8—H8A	0.9900	C23—H23	0.9500
C8—H8B	0.9900	C24—C25	1.370 (4)
C9—C10	1.525 (3)	C24—H24	0.9500
C9—H9A	0.9900	C25—C26	1.394 (3)
C9—H9B	0.9900	C25—H25	0.9500
C10—H10A	0.9900	C26—H26	0.9500
C11—S1—C12	89.42 (10)	N2—C11—S1	121.16 (15)

C1—N1—N2	118.09 (17)	C13—C12—S1	112.95 (15)
C11—N2—N1	111.65 (17)	C13—C12—H12	123.5
C11—N2—H2	121.5	S1—C12—H12	123.5
N1—N2—H2	118.8	C12—C13—N3	112.01 (17)
C11—N3—C13	112.19 (16)	C12—C13—C14	124.63 (17)
C11—N3—C20	122.06 (16)	N3—C13—C14	123.33 (16)
C13—N3—C20	125.56 (15)	C19—C14—C15	119.26 (19)
N1—C1—C2	115.06 (19)	C19—C14—C13	122.95 (18)
N1—C1—C10	125.46 (19)	C15—C14—C13	117.71 (18)
C2—C1—C10	119.48 (18)	C16—C15—C14	119.9 (2)
C3—C2—C7	119.61 (19)	C16—C15—H15	120.0
C3—C2—C1	120.48 (18)	C14—C15—H15	120.0
C7—C2—C1	119.89 (19)	C15—C16—C17	120.2 (2)
C4—C3—C2	120.9 (2)	C15—C16—H16	119.9
C4—C3—H3	119.6	C17—C16—H16	119.9
C2—C3—H3	119.6	C18—C17—C16	120.1 (2)
C3—C4—C5	119.9 (2)	C18—C17—H17	120.0
C3—C4—H4	120.1	C16—C17—H17	120.0
C5—C4—H4	120.1	C17—C18—C19	120.4 (2)
C6—C5—C4	119.7 (2)	C17—C18—H18	119.8
C6—C5—H5	120.2	C19—C18—H18	119.8
C4—C5—H5	120.2	C18—C19—C14	120.1 (2)
C5—C6—C7	121.6 (2)	C18—C19—H19	119.9
C5—C6—H6	119.2	C14—C19—H19	119.9
C7—C6—H6	119.2	N3—C20—C21	113.39 (16)
C6—C7—C2	118.4 (2)	N3—C20—H20A	108.9
C6—C7—C8	121.2 (2)	C21—C20—H20A	108.9
C2—C7—C8	120.42 (19)	N3—C20—H20B	108.9
C7—C8—C9	110.03 (19)	C21—C20—H20B	108.9
C7—C8—H8A	109.7	H20A—C20—H20B	107.7
C9—C8—H8A	109.7	C26—C21—C22	119.5 (2)
C7—C8—H8B	109.7	C26—C21—C20	118.49 (19)
C9—C8—H8B	109.7	C22—C21—C20	121.89 (19)
H8A—C8—H8B	108.2	C23—C22—C21	120.1 (2)
C8—C9—C10	110.9 (2)	C23—C22—H22	120.0
C8—C9—H9A	109.5	C21—C22—H22	120.0
C10—C9—H9A	109.5	C22—C23—C24	120.1 (2)
C8—C9—H9B	109.5	C22—C23—H23	120.0
C10—C9—H9B	109.5	C24—C23—H23	120.0
H9A—C9—H9B	108.0	C25—C24—C23	119.9 (2)
C1—C10—C9	112.50 (18)	C25—C24—H24	120.1
C1—C10—H10A	109.1	C23—C24—H24	120.1
C9—C10—H10A	109.1	C24—C25—C26	120.4 (2)
C1—C10—H10B	109.1	C24—C25—H25	119.8
C9—C10—H10B	109.1	C26—C25—H25	119.8
H10A—C10—H10B	107.8	C21—C26—C25	120.0 (2)
N3—C11—N2	125.43 (18)	C21—C26—H26	120.0
N3—C11—S1	113.41 (14)	C25—C26—H26	120.0

C1—N1—N2—C11	−178.27 (18)	C11—S1—C12—C13	−0.65 (16)
N2—N1—C1—C2	−177.26 (17)	S1—C12—C13—N3	0.0 (2)
N2—N1—C1—C10	2.7 (3)	S1—C12—C13—C14	177.93 (15)
N1—C1—C2—C3	10.0 (3)	C11—N3—C13—C12	0.9 (2)
C10—C1—C2—C3	−170.0 (2)	C20—N3—C13—C12	176.04 (18)
N1—C1—C2—C7	−171.39 (19)	C11—N3—C13—C14	−177.07 (18)
C10—C1—C2—C7	8.6 (3)	C20—N3—C13—C14	−1.9 (3)
C7—C2—C3—C4	−0.8 (3)	C12—C13—C14—C19	125.0 (2)
C1—C2—C3—C4	177.8 (2)	N3—C13—C14—C19	−57.4 (3)
C2—C3—C4—C5	0.1 (3)	C12—C13—C14—C15	−51.8 (3)
C3—C4—C5—C6	0.6 (4)	N3—C13—C14—C15	125.9 (2)
C4—C5—C6—C7	−0.6 (4)	C19—C14—C15—C16	1.5 (3)
C5—C6—C7—C2	−0.2 (4)	C13—C14—C15—C16	178.37 (19)
C5—C6—C7—C8	−178.8 (2)	C14—C15—C16—C17	−0.7 (3)
C3—C2—C7—C6	0.8 (3)	C15—C16—C17—C18	−0.5 (4)
C1—C2—C7—C6	−177.8 (2)	C16—C17—C18—C19	0.9 (4)
C3—C2—C7—C8	179.5 (2)	C17—C18—C19—C14	−0.2 (3)
C1—C2—C7—C8	0.8 (3)	C15—C14—C19—C18	−1.1 (3)
C6—C7—C8—C9	144.2 (2)	C13—C14—C19—C18	−177.76 (19)
C2—C7—C8—C9	−34.4 (3)	C11—N3—C20—C21	−64.4 (2)
C7—C8—C9—C10	58.8 (3)	C13—N3—C20—C21	120.94 (19)
N1—C1—C10—C9	−163.3 (2)	N3—C20—C21—C26	128.1 (2)
C2—C1—C10—C9	16.7 (3)	N3—C20—C21—C22	−55.2 (2)
C8—C9—C10—C1	−50.3 (3)	C26—C21—C22—C23	0.3 (3)
C13—N3—C11—N2	178.69 (19)	C20—C21—C22—C23	−176.3 (2)
C20—N3—C11—N2	3.3 (3)	C21—C22—C23—C24	−0.6 (4)
C13—N3—C11—S1	−1.4 (2)	C22—C23—C24—C25	0.7 (4)
C20—N3—C11—S1	−176.74 (14)	C23—C24—C25—C26	−0.5 (4)
N1—N2—C11—N3	−178.87 (18)	C22—C21—C26—C25	−0.1 (4)
N1—N2—C11—S1	1.2 (2)	C20—C21—C26—C25	176.6 (2)
C12—S1—C11—N3	1.18 (15)	C24—C25—C26—C21	0.2 (4)
C12—S1—C11—N2	−178.90 (18)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···Br1^{i}	0.91	2.63	3.4633 (18)	152
C10—H10*B*···Br1^{i}	0.99	2.88	3.837 (2)	164
C20—H20*B*···Br1^{i}	0.99	2.84	3.7560 (19)	155
C26—H26···Br1^{i}	0.95	2.90	3.730 (2)	146

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

Comparison of pertinent bond lengths and angles (Å, °)

Metric*	I	BOCROC	NUCLOO	QOCGIA
a	1.720 (2)	1.711 (4)	1.7182 (15)	1.740 (2)
b	1.729 (2)	1.740 (4)	1.7373 (15)	1.735 (3)

c	1.419 (2)	1.417 (5)	1.3974 (19)	1.414 (4)
d	1.337 (2)	1.341 (4)	1.3314 (19)	1.373 (4)
e	1.341 (3)	1.329 (5)	1.328 (2)	1.309 (3)
f	1.396 (2)	1.395 (4)	1.3806 (17)	1.381 (3)
g	1.283 (3)	1.275 (5)	1.280 (2)	1.293 (4)
h	121.16 (15)	123.0 (3)	124.94 (11)	126.51 (19)
i	125.43 (18)	123.8 (3)	122.85 (13)	122.3 (2)
j	111.65 (17)	114.9 (3)	117.49 (12)	109.4 (2)
k	118.09 (17)	115.5 (3)	114.40 (13)	116.0 (2)

*Key is **A** in Scheme 2.