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Halogen, chalcogen, and hydrogen bonding in organoiodine cocrystals of heterocyclic thiones: imidazolidine-2-thione, 2-mercaptobenzimidazole, 2-mercapto-5-methylbenzimidazole, 2-mercaptobenzoxazole, and 2-mercaptobenzothiazole

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Spencer Watts, Andrew J. Peloquin, Madhushi Bandara, Colin D. McMillen and William T. Pennington*

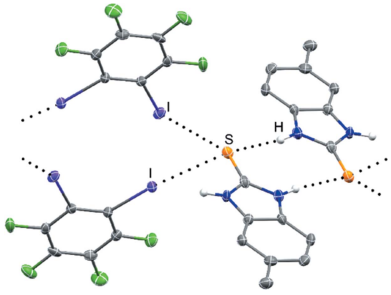
Department of Chemistry, Clemson University, 219 Hunter Laboratories, Clemson, SC 29634, USA. *Correspondence e-mail: billp@clemson.edu

Through the combination of heterocyclic thiones with variation in the identity of the heterocyclic elements, namely, imidazolidine-2-thione, 2-mercaptobenzimidazole, 2-mercapto-5-methylbenzimidazole, 2-mercaptobenzoxazole, and 2-mercaptobenzothiazole with the common halogen-bond donors 1,2-, 1,3-, and 1,4-diiodotetrafluorobenzene, 1,3,5-trifluorotriiodobenzene, and tetraiodoethylene, a series of 18 new crystalline structures were characterized. In most cases, N—H···S hydrogen bonding was observed, with these interactions in imidazole-containing structures typically resulting in two-dimensional motifs (*i.e.* ribbons). Lacking the second N—H group, the thiazole and oxazole hydrogen bonding resulted in only dimeric pairs. C—I···S and C—I···I halogen bonding, as well as C═S···I chalcogen bonding, served to consolidate the packing by linking the hydrogen-bonding ribbons or dimeric pairs.

1. Introduction

Halogen and chalcogen bonding, defined by IUPAC as 'a net attractive interaction between an electrophilic region associated with . . . ' a halogen or chalcogen atom, respectively, ' . . . in a molecular entity and a nucleophilic region in another, or the same, molecular entity (Desiraju *et al.*, 2013; Aakeroy *et al.*, 2019),' has drawn increasing attention in recent years (Parisini *et al.*, 2011; Zhou *et al.*, 2010; Ajani *et al.*, 2015; Arman *et al.*, 2008; Aakeroy *et al.*, 2015; Metrangolo & Resnati, 2012; Cavallo *et al.*, 2016; Metrangolo *et al.*, 2005; Legon, 1998). Similar to hydrogen bonding, halogen bonding is strong, selective, and directional. Organic iodines are among the most commonly utilized halogen-bond donors (Corradi *et al.*, 2000), largely due to their greater polarizability. When paired with halogen-bond acceptor molecules with a diversity of heteroatoms, the combined effects of halogen, chalcogen, and hydrogen bonding can be revealed. Imidazoles, thiazoles, and oxazoles are ideal systems to study in this regard.

Benzimidazole, and its derivatives, have been investigated for a diverse range of biological applications, including in the treatment of tuberculosis (Foks *et al.*, 2006), as antimicrobial agents (Alasmary *et al.*, 2015), and also as analgesic and anti-inflammatory compounds (Achar *et al.*, 2010; Fletcher *et al.*, 2006). These mercaptobenzimidazoles, thiazoles, and oxazoles have also seen significant utilization as ligands in transition-metal complexes. Providing some insight into the role of heteroatoms in differing positions, of the 31 crystal structures



containing 2-mercaptobenzothiazole (**MBZTH**) and a transition metal currently deposited with the Cambridge Structural Database (CSD; Groom *et al.*, 2016), all demonstrate metal coordination through the thione S atom and not the thiazole S atom. They range from simple species, such as (2-mercaptobenzothiazole)bis(triphenylphosphine)silver(I) iodide (Banti *et al.*, 2014), to more complex copper and ruthenium complexes (Zhou *et al.*, 2013*a*; Zafar *et al.*, 2019). Similarly, the mercaptobenzimidazole (or benzimidazolethione) derivatives present an interesting field of study for their potential intermolecular interactions in halogen-bonding systems (Fig. 1). In these systems, hydrogen, halogen, and chalcogen bonding are all viable intermolecular interactions, and structural studies of the cocrystals can be useful in determining which interactions are preferred as the organoiodine and the heterocyclic systems are varied.

Our group has recently been interested in the role of the S atom in I···S halogen- and chalcogen-bonding interactions as a crystal design tool, as well as their roles in the formation of deep eutectic solvents derived from halogen bonding (Peloquin *et al.*, 2021*a*,*b*,*c*,*d*, 2022). Herein, we report the solid-state structures of 18 new cocrystals derived from the combination of the heterocyclic molecules imidazolidine-2-thione (**IT**), 2-mercaptobenzimidazole (**MBZIM**), 2-mercapto-5-methylbenzimidazole (**MMBZIM**), 2-mercaptobenzoxazole (**MBZOX**), and 2-mercaptobenzothiazole (**MBZTH**) with the organic halogen-bond donors 1,2-diiodotetrafluorobenzene (**1,2-F_4DIB**), 1,3-diiodotetrafluorobenzene (**1,3-F_4DIB**), 1,4-tetrafluorobenzene (**1,4-F_4DIB**), 1,3,5-trifluoro-2,4,6-triiodobenzene (**1,3,5-F_3I_3B**), and tetraiodoethylene (**TIE**). This diverse pool of substrates yielded structures with the crystal packing dominated by N—H···S hydrogen bonding, leading to thioamide dimers, with longer-range packing motifs created through C—I···S and C—I···I halogen bonding, as well as the occasional C═S···I chalcogen bond.

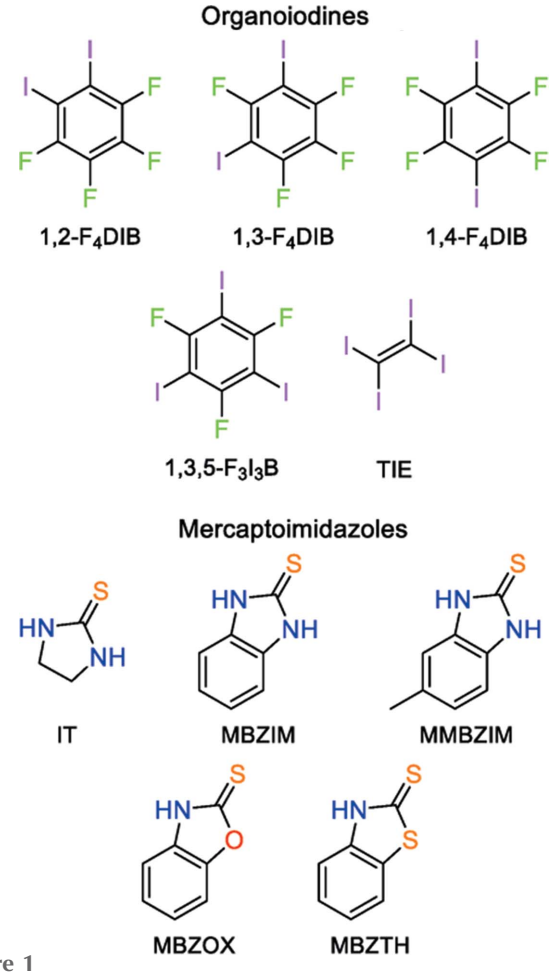


Figure 1
Organoiodines and mercaptoimidazoles utilized in this study.

2. Experimental

2.1. Materials and instrumentation

For single-crystal X-ray analysis, crystals were mounted on low background cryogenic loops using paratone oil. Data were collected using Mo $K\alpha$ radiation (λ = 0.71073 Å) on a Bruker D8 Venture diffractometer with an Incoatec Iμs microfocus source and a Photon 2 detector.

2.2. Preparation of cocrystals

Cocrystals were synthesized using imidazolidine-2-thione (TCI Americas, 98%), 2-mercaptobenzimidazole (Acros, 98%), 2-mercapto-5-methylbenzimidazole (Acros, 99%), 2-mercaptobenzoxazole (Acros, 99%), 2-mercaptobenzothiazole (Acros, 98%), 1,2-diiodotetrafluorobenzene (Synquest Laboratories, 99%), 1,3-diiodotetrafluorobenzene (Synquest Laboratories, 97%), 1,4-tetrafluorobenzene (Synquest Laboratories, 97%), 1,3,5-trifluoro-2,4,6-triiodobenzene (Synquest Laboratories, 99%), and tetraiodoethylene (Santa Cruz Biotechnologies, 98%). Solvents were obtained from Fisher Scientific. All materials were used as received without further purification. Crystals were formed by slow evaporation under ambient conditions (20–23 °C). Methanol was utilized for the majority of cocrystal preparations; however, if this was not successful, acetone or ethyl acetate was utilized.

2.2.1. 2(IT)·(1,3-F_4DIB). Imidazolidine-2-thione (50 mg, 0.489 mmol) and 1,3-diiodotetrafluorobenzene (196 mg, 0.489 mmol) were weighed into a 20 ml glass vial. Methanol (10 ml) was added and the mixture was stirred until a clear solution was obtained. The solvent was allowed to evaporate slowly and colorless needle-like crystals of 2(**IT**)·(**1,3-F_4DIB**) were obtained after 3 d.

2.2.2. (IT)·(1,3,5-F_3I_3B). Imidazolidine-2-thione (50 mg, 0.489 mmol) and 1,3,5-trifluoro-2,4,6-triiodobenzene (249 mg, 0.489 mmol) were weighed into a 20 ml glass vial. Methanol (10 ml) was added and the mixture was stirred until a clear solution was obtained. The solvent was allowed to evaporate slowly and colorless needle-like crystals of (**IT**)·(**1,3,5-F_3I_3B**) were obtained after 4 d.

2.2.3. 4(MBZIM)·3(1,3-F_4DIB). 2-Mercaptobenzimidazole (34 mg, 0.227 mmol) and 1,3-diiodotetrafluorobenzene (49 mg, 0.122 mmol) were weighed into a 20 ml glass vial. Methanol (10 ml) was added and the mixture was stirred until a clear solution was obtained. The solvent was allowed to

Table 1
Experimental details.

Experiments were carried out at 100 K with Mo $K\alpha$ radiation using a Bruker D8 Venture Photon 2 diffractometer. Absorption was corrected for by multi-scan methods (*SADABS*; Bruker, 2017). H atoms were treated by a mixture of independent and constrained refinement, except for 3(**MBZTH**)·4(**1,2-F$_4$DIB**), for which H-atom parameters were constrained.

	2(**IT**)·(**1,3-F$_4$DIB**)	(**IT**)·(**1,3,5-F$_3$I$_3$B**)	4(**MBZIM**)·3(**1,3-F$_4$DIB**)	(**MBZIM**)·(**1,4-F$_4$DIB**)
Crystal data				
Chemical formula	$C_6F_4I_2·2C_3H_6N_2S$	$C_6F_3I_3·C_3H_6N_2S$	$3C_6F_4I_2·4C_7H_6N_2S$	$C_6F_4I_2·C_7H_6N_2S$
M_r	606.18	611.92	1806.37	552.06
Crystal system, space group	Orthorhombic, *Pbcn*	Orthorhombic, *Pbca*	Triclinic, $P\overline{1}$	Monoclinic, $P2_1/c$
a, b, c (Å)	15.6704 (7), 8.9924 (4), 26.0573 (10)	18.0407 (14), 7.2816 (6), 22.1250 (19)	8.4573 (14), 17.725 (3), 18.759 (4)	5.5641 (2), 33.1320 (11), 8.4710 (3)
α, β, γ (°)	90, 90, 90	90, 90, 90	106.997 (7), 93.229 (7), 92.034 (7)	90, 92.754 (1), 90
V (Å^3)	3671.9 (3)	2906.5 (4)	2680.9 (9)	1559.82 (9)
Z	8	8	2	4
μ (mm^{-1})	3.69	6.61	3.72	4.20
Crystal size (mm)	0.18 × 0.17 × 0.13	0.22 × 0.08 × 0.04	0.34 × 0.04 × 0.04	0.22 × 0.18 × 0.06
Data collection				
T_{min}, T_{max}	0.639, 0.746	0.563, 0.746	0.668, 0.746	0.501, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	112821, 5376, 5198	49179, 3615, 3220	118524, 12297, 10558	45583, 4579, 4211
R_{int}	0.035	0.043	0.056	0.050
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.705	0.667	0.651	0.709
Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.015, 0.032, 1.25	0.019, 0.040, 1.11	0.021, 0.041, 1.06	0.020, 0.044, 1.12
No. of reflections	5376	3615	12297	4579
No. of parameters	234	172	717	207
No. of restraints	0	2	8	0
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.42, −0.37	0.57, −0.77	0.52, −0.75	0.49, −0.68

	(**MBZIM**)·(**TIE**)	(**MMBZIM**)·(**1,2-F$_4$DIB**)	2(**MMBZIM**)·(**1,4-F$_4$DIB**)·2(**H$_2$O**)	(**MMBZIM**)·(**1,3,5-F$_3$I$_3$B**)
Crystal data				
Chemical formula	$C_2I_4·C_7H_6N_2S$	$C_6F_4I_2·C_8H_8N_2S$	$C_6F_4I_2·2C_8H_8N_2S·2(H_2O)$	$C_6F_3I_3·C_8H_8N_2S$
M_r	681.82	566.08	766.34	673.98
Crystal system, space group	Orthorhombic, *Pnma*	Triclinic, $P\overline{1}$	Triclinic, $P\overline{1}$	Monoclinic, $P2_1/c$
a, b, c (Å)	11.7547 (10), 8.3525 (7), 15.1077 (13)	4.5504 (5), 13.2872 (14), 13.8064 (14)	4.9088 (3), 11.4670 (8), 11.9686 (8)	15.191 (2), 5.0074 (7), 22.715 (3)
α, β, γ (°)	90, 90, 90	94.766 (4), 98.124 (4), 99.588 (4)	106.644 (2), 98.058 (2), 92.811 (2)	90, 97.460 (6), 90
V (Å^3)	1483.3 (2)	809.97 (15)	636.27 (7)	1713.3 (4)
Z	4	2	1	4
μ (mm^{-1})	8.52	4.05	2.69	5.62
Crystal size (mm)	0.30 × 0.14 × 0.11	0.19 × 0.07 × 0.04	0.31 × 0.11 × 0.08	0.26 × 0.04 × 0.04
Data collection				
T_{min}, T_{max}	0.256, 0.746	0.636, 0.746	0.536, 0.746	0.582, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	32859, 1993, 1885	21426, 3704, 3174	31584, 3558, 3500	23258, 3971, 3039
R_{int}	0.055	0.042	0.036	0.069
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.671	0.650	0.696	0.652
Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.026, 0.062, 1.26	0.026, 0.055, 1.24	0.014, 0.034, 1.18	0.047, 0.105, 1.22
No. of reflections	1993	3704	3558	3971
No. of parameters	89	217	184	217
No. of restraints	0	1	7	1
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.25, −1.48	1.33, −1.06	0.44, −0.42	2.37, −1.89

	(**MBZOX**)·(**1,2-F$_4$DIB**)	(**MBZOX**)·(**1,3-F$_4$DIB**)	2(**MBZOX**)·(**1,4-F$_4$DIB**)	(**MBZOX**)·(**1,3,5-F$_3$I$_3$B**)
Crystal data				
Chemical formula	$C_6F_4I_2·C_7H_5NOS$	$C_6F_4I_2·C_7H_5NOS$	$C_6F_4I_2·2C_7H_5NOS$	$C_6F_3I_3·C_7H_5NOS$
M_r	553.04	553.04	704.22	660.94
Crystal system, space group	Monoclinic, $P2_1/n$	Monoclinic, $P2_1/c$	Monoclinic, $C2/c$	Monoclinic, $P2_1/c$

Table 1 (continued)

	(**MBZOX**)·(**1,2-F$_4$DIB**)	(**MBZOX**)·(**1,3-F$_4$DIB**)	2(**MBZOX**)·(**1,4-F$_4$DIB**)	(**MBZOX**)·(**1,3,5-F$_3$I$_3$B**)
a, *b*, *c* (Å)	13.7789 (12), 4.4129 (4), 25.252 (2)	15.1655 (8), 4.3803 (2), 23.0358 (12)	31.025 (4), 4.3159 (5), 19.061 (2)	14.9295 (7), 4.6119 (2), 23.5065 (12)
α, β, γ (°)	90, 96.337 (3), 90	90, 99.923 (2), 90	90, 114.434 (4), 90	90, 92.548 (2), 90
V (Å^3)	1526.0 (2)	1507.36 (13)	2323.6 (5)	1616.90 (13)
Z	4	4	4	4
μ (mm^{-1})	4.30	4.35	2.94	5.96
Crystal size (mm)	0.46 × 0.06 × 0.02	0.23 × 0.12 × 0.09	0.29 × 0.12 × 0.03	0.22 × 0.06 × 0.05
Data collection				
T_{min}, T_{max}	0.578, 0.745	0.541, 0.746	0.637, 0.746	0.551, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12498, 3210, 2510	39610, 4625, 4119	25197, 2950, 2571	19413, 3348, 2845
R_{int}	0.066	0.042	0.047	0.050
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.634	0.716	0.675	0.630
Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.047, 0.087, 1.11	0.022, 0.048, 1.16	0.028, 0.060, 1.32	0.029, 0.061, 1.22
No. of reflections	3210	4625	2950	3348
No. of parameters	203	203	149	203
No. of restraints	0	0	0	0
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.58, −1.52	0.96, −1.35	1.54, −1.15	0.80, −0.77

	3(**MBZTH**)·4(**1,2-F$_4$DIB**)	(**MBZTH**)·(**1,3-F$_4$DIB**)	(**MBZTH**)·2(**1,3-F$_4$DIB**)	2(**MBZTH**)·(**1,4-F$_4$DIB**)
Crystal data				
Chemical formula	$4C_6F_4I_2{\cdot}3C_7H_5NS_2$	$C_6F_4I_2{\cdot}C_7H_5NS_2$	$4C_6F_4I_2{\cdot}2C_7H_5NS_2$	$C_6F_4I_2{\cdot}2C_7H_5NS_2$
M_r	2109.16	569.10	1941.92	736.34
Crystal system, space group	Triclinic, $P\overline{1}$	Triclinic, $P\overline{1}$	Monoclinic, $P2_1$	Monoclinic, $P2_1/n$
a, *b*, *c* (Å)	7.9410 (8), 14.8483 (15), 24.641 (3)	7.2175 (4), 8.2675 (5), 14.4498 (9)	4.5581 (3), 34.358 (2), 15.6075 (10)	5.5057 (2), 15.6087 (7), 13.5194 (6)
α, β, γ (°)	79.264 (4), 87.104 (4), 82.784 (4)	97.936 (2), 91.297 (2), 109.178 (2)	90, 94.707 (2), 90	90, 94.259 (2), 90
V (Å^3)	2830.9 (5)	804.44 (8)	2436.0 (3)	1158.61 (8)
Z	2	2	2	2
μ (mm^{-1})	4.69	4.20	5.36	3.12
Crystal size (mm)	0.30 × 0.13 × 0.04	0.33 × 0.27 × 0.06	0.18 × 0.12 × 0.04	0.17 × 0.09 × 0.04
Data collection				
T_{min}, T_{max}	0.570, 0.746	0.496, 0.746	0.568, 0.746	0.559, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	78566, 12466, 11325	27899, 4701, 4391	56285, 12660, 11766	22270, 3402, 2811
R_{int}	0.067	0.036	0.050	0.049
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.642	0.706	0.678	0.706
Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.067, 0.220, 1.06	0.018, 0.044, 1.09	0.026, 0.046, 1.09	0.027, 0.057, 1.15
No. of reflections	12466	4701	12660	3402
No. of parameters	704	203	622	149
No. of restraints	66	0	2	0
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	2.61, −1.48	1.08, −1.11	1.01, −0.71	0.90, −0.79
Absolute structure	–	–	Refined as an inversion twin	–
Absolute structure parameter	–	–	0.454 (15)	–

	(**MBZTH**)·(**1,3,5-F$_3$I$_3$B**)	(**MBZTH**)·(**TIE**)
Crystal data		
Chemical formula	$C_6F_3I_3{\cdot}C_7H_5NS_2$	$C_2I_4{\cdot}C_7H_5NS_2$
M_r	677.00	698.86
Crystal system, space group	Monoclinic, $P2_1/c$	Triclinic, $P\overline{1}$
a, *b*, *c* (Å)	15.2665 (6), 4.7380 (2), 23.2215 (10)	7.4085 (6), 10.8180 (9), 11.1989 (10)
α, β, γ (°)	90, 93.139 (2), 90	66.616 (3), 70.765 (3), 70.792 (3)
V (Å^3)	1677.15 (12)	757.20 (11)
Z	4	2
μ (mm^{-1})	5.86	8.48
Crystal size (mm)	0.16 × 0.08 × 0.05	0.08 × 0.07 × 0.07
Data collection		
T_{min}, T_{max}	0.610, 0.746	0.589, 0.746

Table 1 (continued)

	(MBZTH)·(1,3,5-F_3I_3B)	(MBZTH)·(TIE)
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	35222, 4212, 3611	22463, 3484, 3037
R_{int}	0.057	0.052
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.669	0.651
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.024, 0.052, 1.18	0.029, 0.072, 1.13
No. of reflections	4212	3484
No. of parameters	203	159
No. of restraints	1	7
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.67, −0.73	1.43, −1.76

computer programs: *APEX3* (Bruker, 2017), *SAINT* (Bruker, 2017), *SHELXT2018* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*), *Mercury* (Macrae *et al.*, 2020), and *OLEX2* (Dolomanov *et al.*, 2009).

evaporate slowly and colorless needle-like crystals of 4(**MBZIM**)·3(**1,3-F_4DIB**) were obtained after 4 d.

2.2.4. (MBZIM)·(1,4-F_4DIB). 2-Mercaptobenzimidazole (19 mg, 0.126 mmol) and 1,4-diiodotetrafluorobenzene (50 mg, 0.124 mmol) were weighed into a 20 ml glass vial. Methanol (10 ml) was added and the mixture was stirred until a clear solution was obtained. The solvent was allowed to evaporate slowly and colorless plate-like crystals of (**MBZIM**)·(**1,4-F_4DIB**) were obtained after 3 d.

2.2.5. (MBZIM)·(TIE). 2-Mercaptobenzimidazole (30 mg, 0.200 mmol) and tetraiodoethylene (55 mg, 0.103 mmol) were weighed into a 20 ml glass vial. Ethyl acetate (15 ml) was added and the mixture was stirred until a clear solution was obtained. The solvent was allowed to evaporate slowly and colorless tabular crystals of (**MBZIM**)·(**TIE**) were obtained after 7 d.

2.2.6. (MMBZIM)·(1,2-F_4DIB). 2-Mercapto-5-methylbenzimidazole (20 mg, 0.122 mmol) and 1,2-diiodotetrafluorobenzene (48 mg, 0.119 mmol) were weighed into a 20 ml glass vial. Methanol (10 ml) was added and the mixture was stirred until a clear solution was obtained. The solvent was allowed to evaporate slowly and colorless columnar crystals of (**MMBZIM**)·(**1,2-F_4DIB**) were obtained after 3 d.

2.2.7. 2(MMBZIM)·(1,4-F_4DIB)·2(H_2O). 2-Mercapto-5-methylbenzimidazole (40 mg, 0.244 mmol) and 1,4-diiodotetrafluorobenzene (51 mg, 0.127 mmol) were weighed into a 20 ml glass vial. Methanol (10 ml) was added and the mixture was stirred until a clear solution was obtained. The solvent was allowed to evaporate slowly and colorless plate-like crystals of 2(**MMBZIM**)·(**1,4-F_4DIB**)·2(**H_2O**) were obtained after 3 d.

2.2.8. (MMBZIM)·(1,3,5-F_3I_3B). 2-Mercapto-5-methylbenzimidazole (31 mg, 0.189 mmol) and 1,3,5-trifluoro-2,4,6-triiodobenzene (50 mg, 0.098 mmol) were weighed into a 20 ml glass vial. Methanol (10 ml) was added and the mixture was stirred until a clear solution was obtained. The solvent was allowed to evaporate slowly and colorless needle-like crystals of (**MMBZIM**)·(**1,3,5-F_3I_3B**) were obtained after 4 d.

2.2.9. (MBZOX)·(1,2-F_4DIB). 2-Mercaptobenzoxazole (20 mg, 0.132 mmol) and 1,2-diiodotetrafluorobenzene (102 mg, 0.254 mmol) were weighed into a 20 ml glass vial. Methanol (10 ml) was added and the mixture was stirred until a clear solution was obtained. The solvent was allowed to evaporate slowly and colorless needle-like crystals of (**MBZOX**)·(**1,2-F_4DIB**) were obtained after 3 d.

2.2.10. (MBZOX)·(1,3-F_4DIB). 2-Mercaptobenzoxazole (19 mg, 0.126 mmol) and 1,3-diiodotetrafluorobenzene (104 mg, 0.259 mmol) were weighed into a 20 ml glass vial. Acetone (10 ml) was added and the mixture was stirred until a clear solution was obtained. The solvent was allowed to evaporate slowly and colorless columnar crystals of (**MBZOX**)·(**1,3-F_4DIB**) were obtained after 2 d.

2.2.11. 2(MBZOX)·(1,4-F_4DIB). 2-Mercaptobenzoxazole (40 mg, 0.265 mmol) and 1,4-diiodotetrafluorobenzene (50 mg, 0.124 mmol) were weighed into a 20 ml glass vial. Acetone (10 ml) was added and the mixture was stirred until a clear solution was obtained. The solvent was allowed to evaporate slowly and colorless columnar crystals of 2(**MBZOX**)·(**1,4-F_4DIB**) were obtained after 2 d.

2.2.12. (MBZOX)·(1,3,5-F_3I_3B). 2-Mercaptobenzoxazole (15 mg, 0.099 mmol) and 1,3,5-trifluoro-2,4,6-triiodobenzene (50 mg, 0.098 mmol) were weighed into a 20 ml glass vial. Acetone (10 ml) was added and the mixture was stirred until a clear solution was obtained. The solvent was allowed to evaporate slowly and colorless columnar crystals of (**MBZOX**)·(**1,3,5-F_3I_3B**) were obtained after 1 d.

2.2.13. 3(MBZTH)·4(1,2-F_4DIB). 2-mercaptobenzothiazole (21 mg, 0.126 mmol) and 1,2-diiodotetrafluorobenzene (103 mg, 0.256 mmol) were weighed into a 20 ml glass vial. Methanol (10 ml) was added and the mixture was stirred until a clear solution was obtained. The solvent was allowed to evaporate slowly and colorless plate-like crystals of 3(**MBZTH**)·4(**1,2-F_4DIB**) were obtained after 3 d.

2.2.14. (MBZTH)·(1,3-F_4DIB). 2-Mercaptobenzothiazole (24 mg, 0.143 mmol) and 1,3-diiodotetrafluorobenzene (50 mg, 0.124 mmol) were weighed into a 20 ml glass vial. Methanol (10 ml) was added and the mixture was stirred until a clear solution was obtained. The solvent was allowed to evaporate slowly and colorless plate-like crystals of (**MBZTH**)·(**1,3-F_4DIB**) were obtained after 3 d.

2.2.15. (MBZTH)·2(1,3-F_4DIB). 2-Mercaptobenzothiazole (22 mg, 0.132 mmol) and 1,3-diiodotetrafluorobenzene (98 mg, 0.244 mmol) were weighed into a 20 ml glass vial. Methanol (10 ml) was added and the mixture was stirred until a clear

Table 2
Hydrogen-bond geometry (Å, °) for 2(**IT**)·(**1,3-F$_4$DIB**).

D—H···A	D—H	H···A	D···A	D—H···A
N1—HN1···S1^{i}	0.81 (2)	2.77 (2)	3.5551 (14)	163 (2)
N2—HN2···S2^{ii}	0.83 (2)	2.53 (2)	3.3507 (14)	172 (2)
C2—H2B···F2	0.99	2.55	3.3392 (19)	136
C3—H3B···S2	0.99	2.94	3.7351 (19)	138
N3—HN3···S2^{iii}	0.79 (2)	2.54 (2)	3.3171 (15)	167 (2)
N4—HN4···I2^{iv}	0.83 (2)	3.31 (2)	3.7383 (14)	114.9 (18)
N4—HN4···S1^{ii}	0.83 (2)	2.63 (2)	3.4562 (14)	179 (2)
C5—H5A···I1^{v}	0.99	3.20	3.9922 (16)	138
C5—H5B···F4	0.99	2.45	3.2774 (19)	140
C6—H6B···I1^{vi}	0.99	3.18	3.9223 (16)	133

Symmetry codes: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, z$; (ii) $-x+1, -y+2, -z+1$; (iii) $-x+1, -y+1, -z+1$; (iv) $-x+\frac{3}{2}, y+\frac{1}{2}, z$; (v) $-x+1, y, -z+\frac{1}{2}$; (vi) $x-\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.

solution was obtained. The solvent was allowed to evaporate slowly and colorless tabular crystals of (**MBZTH**)·2(**1,3-F$_4$DIB**) were obtained after 4 d.

2.2.16. 2(MBZTH)·(1,4-F$_4$DIB). 2-Mercaptobenzothiazole (46 mg, 0.275 mmol) and 1,4-diiodotetrafluorobenzene (50 mg, 0.124 mmol) were weighed into a 20 ml glass vial. Acetone (10 ml) was added and the mixture was stirred until a clear solution was obtained. The solvent was allowed to evaporate slowly and colorless needle-like crystals of 2(**MBZTH**)·(**1,4-F$_4$DIB**) were obtained after 2 d.

2.2.17. (MBZTH)·(1,3,5-F$_3$I$_3$B). 2-Mercaptobenzothiazole (32 mg, 0.191 mmol) and 1,3,5-trifluoro-2,4,6-triiodobenzene (50 mg, 0.098 mmol) were weighed into a 20 ml glass vial. Acetone (10 ml) was added and the mixture was stirred until a clear solution was obtained. The solvent was allowed to evaporate slowly and colorless tabular crystals of (**MBZTH**)·(**1,3,5-F$_3$I$_3$B**) were obtained after 2 d.

2.2.18. (MBZTH)·(TIE). 2-Mercaptobenzothiazole (33 mg, 0.197 mmol) and tetraiodoethylene (50 mg, 0.094 mmol) were weighed into a 20 ml glass vial. Methanol (15 ml) was added and the mixture was stirred with gentle heating until a clear solution was obtained. The solvent was allowed to evaporate slowly and colorless block-like crystals of (**MBZTH**)·(**TIE**) were obtained after 5 d.

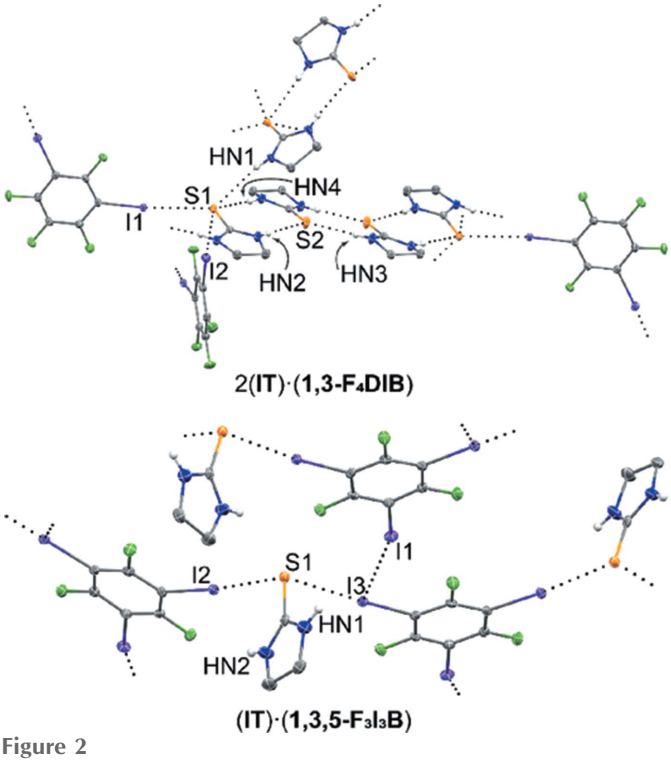


Figure 2
Cocrystalline structures containing **IT**. Hydrogen and halogen bonding are indicated by black dotted lines. Displacement ellipsoids are drawn at the 50% probability level. H atoms, except those bound to N atoms, have been omitted for clarity.

2.3. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. H atoms on C atoms were calculated in idealized positions riding on their parent atoms, with C—H = 0.98 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms, and C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C) for other H atoms. H atoms on heteroatoms were located in difference Fourier maps and refined isotropically, utilizing appropriate restraints [N—H = 0.86 (2) Å] where necessary to maintain chemically reasonable geometries. The H atoms of the water molecule in 2(**MMBZIM**)·(**1,4-F$_4$DIB**)·2(**H$_2$O**) were modeled in a disordered arrangement due to symmetry considerations.

3. Results and discussion

3.1. Cocrystals of imidazolidine-2-thione (IT)

The smallest of the sulfur-containing compounds within this study, imidazolidine-2-thione, contains a thiourea functionality within a five-membered saturated ring. The first cocrystal formed with this compound in the present study is 2(**IT**)·(**1,3-F$_4$DIB**), which was refined in the orthorhombic space group *Pbcn* with two unique molecules of **IT** and one molecule of **1,3-F$_4$DIB** in the asymmetric unit (Fig. 2). As is common in thiourea-containing structures, a pair of N—H···S hydrogen bonds links thiourea molecules, in this case, into tetrameric units (Table 2) (Peloquin *et al.*, 2021*d*, 2022). This is in contrast to the formation of hydrogen-bonded ribbons and discrete dimers, which are formed in the previously published 2(**IT**)·(**1,2-F$_4$DIB**) and (**IT**)·2(**1,2-F$_4$DIB**) cocrystals, respectively (Happonen *et al.*, 2021). Tetrameric units align into staggered stacks in the *b* direction. These stacks are separated by additional tetrameric units, with the planes of the tetramers inclined by approximately 64°. This arrangement of inclined hydrogen-bonding units is also observed in the dimeric units of (**IT**)·(**1,4-F$_4$DIB**) (Happonen *et al.*, 2021). At the end of each tetramer, the remaining N—H hydrogen serves to link to the next inclined tetramer *via* N—H···S hydrogen bonding. The S atom at this end, S1, acts as a C—I···S halogen-bond acceptor to two different **1,3-F$_4$DIB** molecules (Table 3). These halogen-bonding interactions link adjacent stacks of tetramers in the *c* direction. The second **IT**-containing cocrystal of this study, (**IT**)·(**1,3,5-F$_3$I$_3$B**), was refined in the orthorhombic space group *Pbca* with one molecule each of **IT** and **1,3,5-F$_3$I$_3$B** in the asymmetric unit. This structure represents the only example within this study without N—H···S

Table 3
Halogen- and chalcogen-bond geometries (Å, °).

Compound		$d(D\cdots A)$	R_{XB}[i]	$\theta(C-D\cdots A)$	$\theta(D\cdots A-C)$	$\theta_1-\theta_2$[ii]	ψ[iii]
2(**IT**)·(**1,3-F$_4$DIB**)	I1···S1	3.2265 (6)	0.85	174.51 (4)	113.51 (5)	61.00	0.79
	I2···S1	3.2860 (5)	0.87	176.10 (4)	99.67 (5)	76.43	0.03
(**IT**)·(**1,3,5-F$_3$I$_3$B**)	I1···I3	3.8376 (6)	0.97	162.95 (8)	106.24 (7)	56.71	0.64
	I2···S1	3.1505 (8)	0.83	171.86 (7)	101.89 (10)	69.97	0.48
	I3···S1	3.1754 (8)	0.84	177.68 (8)	90.59 (9)	87.09	0.18
4(**MBZIM**)·3(**1,3-F$_4$DIB**)	I1···S3	3.3361 (10)	0.88	172.18 (8)	136.86 (8)	35.32	0.83
	I6···S2	3.2150 (9)	0.85	166.06 (8)	134.24 (8)	31.82	0.74
(**MBZIM**)·(**1,4-F$_4$DIB**)	I1···S1	3.2573 (9)	0.86	168.29 (6)	131.28 (8)	37.01	0.57
(**MBZIM**)·(**TIE**)	I1···S1	3.5368 (14)	0.94	173.83 (17)	71.37 (16)	102.46	0.66
	I3···S1	3.2702 (14)	0.87	177.05 (17)	118.15 (17)	58.90	0.64
(**MMBZIM**)·(**1,2-F$_4$DIB**)	I1···S1	3.6404 (10)	0.96	154.63 (12)	95.76 (13)	58.87	0.47
	I2···S1	3.2307 (11)	0.85	169.63 (11)	106.66 (15)	62.97	0.04
2(**MMBZIM**)·(**1,4-F$_4$DIB**)·2(**H$_2$O**)	I1···S1	3.2516 (4)	0.86	169.16 (4)	96.12 (4)	73.04	0.37
(**MMBZIM**)·(**1,3,5-F$_3$I$_3$B**)	I2···S1	3.474 (2)	0.92	164.1 (3)	92.1 (3)	72.0	0.71
	I3···S1	3.463 (2)	0.92	176.7 (3)	96.5 (3)	80.2	0.50
(**MBZOX**)·(**1,2-F$_4$DIB**)	I2···S1	3.2853 (19)	0.87	166.65 (19)	105.4 (3)	61.3	0.19
(**MBZOX**)·(**1,3-F$_4$DIB**)	I1···S1	3.4132 (7)	0.90	174.53 (6)	105.63 (8)	68.90	0.19
	I2···S1	3.6787 (6)	0.97	159.40 (6)	92.48 (7)	66.92	0.66
	S1···I1	3.7536 (7)	0.99	160.34 (7)	105.80 (6)	54.54	0.53
2(**MBZOX**)·(**1,4-F$_4$DIB**)	I1···S1	3.2287 (11)	0.85	174.60 (9)	109.39 (13)	65.21	0.74
(**MBZOX**)·(**1,3,5-F$_3$I$_3$B**)	I1···S1	3.4114 (14)	0.90	171.55 (13)	100.14 (19)	71.41	0.14
	I2···I3	3.9110 (7)	0.99	147.22 (13)	79.55 (13)	67.67	0.62
	I3···S1	3.6774 (13)	0.97	157.67 (15)	95.79 (16)	61.88	0.67
	S1···I1	3.7385 (14)	0.99	163.12 (17)	98.99 (14)	64.13	0.44
3(**MBZTH**)·4(**1,2-F$_4$DIB**)	I1···S5	3.380 (4)	0.89	177.9 (4)	113.3 (5)	64.6	0.81
	I2···S5	3.353 (4)	0.89	163.7 (4)	128.9 (5)	34.8	0.61
	I3···S3	3.371 (5)	0.89	169.0 (4)	96.4 (7)	72.6	0.02
	I4···S3	3.754 (4)	0.99	173.7 (4)	100.5 (6)	73.2	0.76
	I5···S1	3.380 (4)	0.89	177.9 (4)	113.3 (5)	64.6	0.81
	I6···I7	3.8766 (14)	0.95	170.5 (4)	118.1 (4)	52.4	0.73
	I6···S1	3.391 (5)	0.90	168.1 (4)	111.3 (6)	56.8	0.76
(**MBZTH**)·(**1,3-F$_4$DIB**)	I1···S1	3.3724 (5)	0.89	168.06 (6)	120.18 (6)	47.88	0.64
	I2···S1	3.4140 (5)	0.90	157.68 (4)	106.00 (5)	51.68	0.66
(**MBZTH**)·2(**1,3-F$_4$DIB**)	I1···S3	3.3426 (17)	0.88	168.34 (18)	103.3 (2)	65.0	0.25
	I2···S2	3.7429 (17)	0.99	152.94 (18)	121.7 (4)[iii]	31.2	0.23
	I3···S1	3.3548 (18)	0.89	166.60 (17)	100.3 (2)	66.3	0.64
	I4···S4	3.6744 (17)	0.97	148.74 (18)	118.4 (4)[iii]	30.4	0.65
	I5···I4	3.7971 (10)	0.96	163.30 (19)	82.92 (18)	80.38	0.52
	I8···I2	3.7950 (9)	0.96	170.03 (18)	84.69 (18)	85.34	0.71
2(**MBZTH**)·(**1,4-F$_4$DIB**)	I1···S1	3.3013 (7)	0.87	178.16 (7)	103.84 (10)	74.32	0.60
(**MBZTH**)·(**1,3,5-F$_3$I$_3$B**)	I1···S1	3.4551 (10)	0.91	169.01 (9)	97.89 (13)	71.12	0.71
	S2···I3	3.7777 (10)	1.00	158.73 (12)	117.64 (10)	41.09	0.52
(**MBZTH**)·(**TIE**)	I1···I3	3.9459 (7)	1.00	171.07 (14)	70.7 (3)	100.4	0.55
	I3···S1	3.2826 (13)	0.87	162.1 (3)	122.51 (19)	39.6	0.41
	I4···S1	3.6514 (19)	0.97	161.9 (3)	77.0 (2)	84.9	0.46

Notes: (i) $R_{XB} = d(X\cdots Y)/\Sigma d(\text{vdW})$, the ratio of the distance between the donor atom (*i.e.* I) and the acceptor atom (*i.e.* S) to the sum of their van der Waals (vdW) radii (S = 1.80 Å and I = 1.98 Å) (Auffinger *et al.*, 2004). (ii) $\theta_1-\theta_2 = |[[\theta(C-D\cdots A)] - [\theta(D\cdots A-C)]]|$. (iii) Linearity parameter (Setter *et al.*, 2020).

hydrogen bonding (Table 4). Instead, C—I···S halogen bonding occurs between alternating molecules of **IT** and **1,3,5-F$_3$I$_3$B** to form chains propagating in the *c* direction. The third I atom of **1,3,5-F$_3$I$_3$B**, which does not participate in significant interactions with sulfur, instead serves to link chains in the *ac* plane *via* C—I···I halogen bonding.

3.2. Cocrystals of 2-mercaptobenzimidazole (MBZIM)

Moving to the larger thiourea-containing molecule 2-mercaptobenzimidazole (**MBZIM**) yielded three new structures dominated by co-operative hydrogen and halogen bonding (Fig. 3). With **1,3-F$_4$DIB**, the cocrystalline structure of 4(**MBZIM**)·3(**1,3-F$_4$DIB**) was obtained in the triclinic space group $P\overline{1}$, with four unique molecules of **MBZIM** and three molecules of **1,3-F$_4$DIB** in the asymmetric unit. In this structure, hydrogen bonding between thiourea molecules contributes to the formation of ribbons propagating along the *a* axis (Table 5). Two of the three **1,3-F$_4$DIB** molecules are pendants along these chains, linked *via* C—I···S. The second I atom of these particular **1,3-F$_4$DIB** molecules does not contribute to significant halogen- or chalcogen-bonding interactions. This

Table 4
Hydrogen-bond geometry (Å, °) for (**IT**)·(**1,3,5-F$_3$I$_3$B**).

D—H···A	D—H	H···A	$D\cdots A$	D—H···A
N2—HN2···I2^{i}	0.83 (2)	3.10 (3)	3.742 (3)	137 (3)
C2—H2B···I1^{ii}	0.99	3.31	3.927 (3)	122
C2—H2B···F3^{iii}	0.99	2.47	3.147 (3)	125

Symmetry codes: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, z$; (ii) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$; (iii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.

hydrogen-bonding thiourea ribbon with halogen-bonding pendants is analogous to that observed in (**MBZIM**)·(**1,2-F$_4$DIB**) (Arman *et al.*, 2008, 2010). The final unique **1,3-F$_4$DIB** molecule lies between the ring planes of the pendant molecules of **1,3-F$_4$DIB**, contributing to only weak C—I···H, C—F···H, and C—F···F—C interactions. The combination of **MBZIM** and **1,4-F$_4$DIB** resulted in the (**MBZIM**)·(**1,4-F$_4$DIB**) cocrystal, refined in the monoclinic space group $P2_1/c$, with one molecule each of both **MBZIM** and **1,4-F$_4$DIB** in the asymmetric unit. Just as in 4(**MBZIM**)·3(**1,3-F$_4$DIB**), the structure of (**MBZIM**)·(**1,4-F$_4$DIB**) consists of ribbons of **MBZIM** molecules propagating in the *c* direction, formed through thiourea hydrogen bonding (Table 6). Molecules of

Table 5
Hydrogen-bond geometry (Å, °) for 4(**MBZIM**)·3(**1,3-F$_4$DIB**).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—HN1···S2^{i}	0.85 (2)	2.52 (2)	3.357 (2)	172 (3)
N2—HN2···S2	0.85 (2)	2.46 (2)	3.297 (2)	166 (2)
N3—HN3···S1	0.85 (2)	2.51 (2)	3.348 (2)	173 (3)
N4—HN4···S1^{ii}	0.85 (2)	2.50 (2)	3.326 (2)	166 (2)
N5—HN5···S4^{i}	0.85 (2)	2.49 (2)	3.326 (2)	169 (3)
N6—HN6···S4	0.85 (2)	2.43 (2)	3.270 (2)	169 (3)
C17—H17···F36^{iii}	0.95	2.61	3.385 (3)	139
C20—H20···F36^{iv}	0.95	2.51	3.235 (3)	133
N7—HN7···S3	0.84 (2)	2.47 (2)	3.300 (2)	170 (3)
N8—HN8···S3^{ii}	0.85 (2)	2.48 (2)	3.302 (2)	163 (3)

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

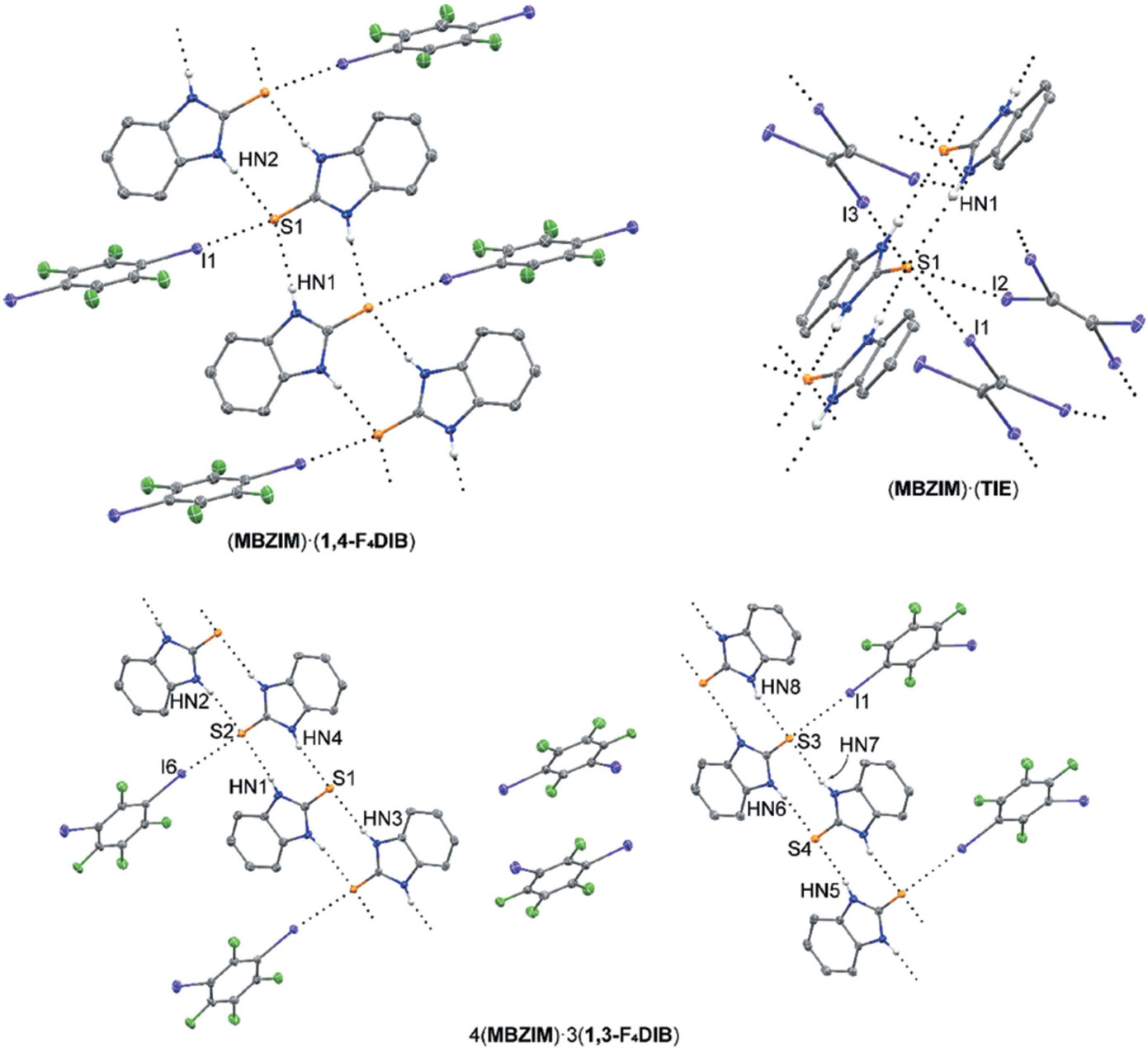


Figure 3
Cocrystal structures containing **MBZIM**. Hydrogen and halogen bonding are indicated by black dotted lines. Displacement ellipsoids are drawn at the 50% probability level. H atoms, except those bound to N atoms, have been omitted for clarity.

Table 6
Hydrogen-bond geometry (Å, °) for (**MBZIM**)·(**1,4-F$_4$DIB**).

D—H···A	D—H	H···A	D···A	D—H···A
N1—HN1···S1^{i}	0.84 (3)	2.47 (3)	3.3089 (18)	172 (2)
N2—HN2···S1^{ii}	0.86 (3)	2.50 (3)	3.3527 (17)	172 (2)

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

Table 7
Hydrogen-bond geometry (Å, °) for (**MBZIM**)·(**TIE**).

D—H···A	D—H	H···A	D···A	D—H···A
N1—HN1···S1^{i}	0.87 (5)	2.47 (5)	3.335 (3)	178 (5)
C3—H3···I1^{ii}	0.95	3.28	3.881 (4)	123

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $-x+\frac{3}{2}, -y+1, z+\frac{1}{2}$.

Table 8
Hydrogen-bond geometry (Å, °) for (**MMBZIM**)·(**1,2-F$_4$DIB**).

D—H···A	D—H	H···A	D···A	D—H···A
N1—HN1···S1^{i}	0.88 (5)	2.57 (5)	3.444 (3)	173 (4)
N2—HN2···I1	0.85 (2)	3.07 (3)	3.780 (3)	142 (3)
N2—HN2···F4	0.85 (2)	2.56 (3)	3.122 (4)	124 (3)
C3—H3···I2^{ii}	0.95	3.06	3.966 (4)	160
C6—H6···F4	0.95	2.63	3.262 (4)	125

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

1,4-F$_4$DIB act as pendants along these ribbons, linked *via* C—I···S halogen bonding.

With four I atoms available, tetraiodoethylene (**TIE**) often enables structural motifs that are different from the typical aromatic halogen-bond donors. The cocrystal (**MBZIM**)·(**TIE**) was refined in the orthorhombic space group *Pnma*, with one molecule each of **MBZIM** and **TIE** in the asymmetric unit. As in the previous examples, molecules of **MBZIM** form infinite ribbons through thiourea hydrogen bonding (Table 7). Three of the four I atoms of **TIE** function as C—I···S halogen-bond donor atoms to link these ribbons, creating a three-dimensional framework through the combination of hydrogen and halogen bonding. The fourth I atom participates in a C—I···π interaction [I···π = 3.351 (3) Å] to reinforce the framework.

3.3. Cocrystals of 2-mercapto-5-methylbenzimidazole (MMBZIM)

Adding a methyl group to **MBZIM**, resulting in 2-mercapto-5-methylbenzimidazole (**MMBZIM**), induces significant changes to the overall hydrogen- and halogen-bonding motifs. The structural literature of this substrate is limited, having only been characterized by single-crystal X-ray diffraction when acting as a ligand for transition metals coordinating through its S atom (Lin *et al.*, 2017; Ozturk *et al.*, 2009; Mitra *et al.*, 2012). The first halogen-bonded cocrystal of **MMBZIM** in this study, (**MMBZIM**)·(**1,2-F$_4$DIB**), was refined in the triclinic space group $P\overline{1}$, with one molecule each of **MMBZIM** and **1,2-F$_4$DIB** in the asymmetric unit (Fig. 4). A discrete hydrogen-bonded dimer of two **MMBZIM** molecules is observed, in contrast to the infinite ribbons in (**MBZIM**)·(**1,2-F$_4$DIB**) and most of the cocrystals in the present study (Table 8). Two molecules of **1,2-F$_4$DIB** per **MMBZIM** molecule link the dimers *via* C—I···S halogen bonds, leading to the formation of chains along the *c* axis.

Isolated as a hydrated cocrystal from adventitious water, 2(**MMBZIM**)·(**1,4-F4DIB**)·2(**H$_2$O**) crystallizes in the triclinic space group $P\overline{1}$ with one molecule each of **MMBZIM** and **H$_2$O**, as well as half a molecule of **1,4-F$_4$DIB**, in the asymmetric unit. All attempts to obtain an nonhydrated cocrystal

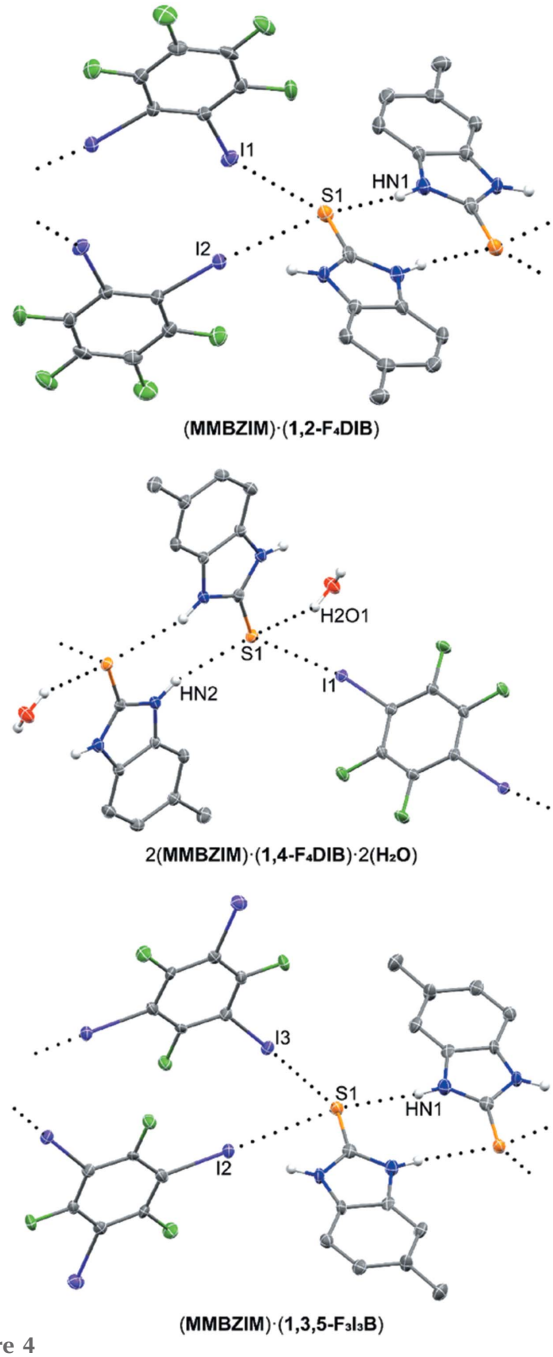


Figure 4
Cocrystalline structures containing **MMBZIM**. Hydrogen and halogen bonding are indicated by black dotted lines. Displacement ellipsoids are drawn at the 50% probability level. H atoms, except those bound to N atoms, have been omitted for clarity.

Table 9
Hydrogen-bond geometry (Å, °) for 2(**MMBZIM**)·(**1,4-F$_4$DIB**)·2(**H$_2$O**).

D—H···A	D—H	H···A	D···A	D—H···A
N1—HN1···O1	0.83 (2)	2.06 (2)	2.8763 (17)	166 (2)
N2—HN2···S1^{i}	0.88 (2)	2.57 (2)	3.4211 (13)	164 (2)
C4—H4···I1^{ii}	0.95	3.03	3.9505 (14)	164
O1—H1*A*O···O1^{iii}	0.88 (2)	1.85 (2)	2.708 (3)	163 (4)
O1—H1*B*O···O1^{iv}	0.88 (2)	1.89 (2)	2.759 (3)	167 (4)
O1—H2O1···I1	0.87 (2)	3.16 (3)	3.7419 (12)	126 (2)
O1—H2O1···S1^{iii}	0.87 (2)	2.65 (2)	3.4251 (13)	149 (3)

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

Table 10
Hydrogen-bond geometry (Å, °) for (**MMBZIM**)·(**1,3,5-F$_3$I$_3$B**).

D—H···A	D—H	H···A	D···A	D—H···A
N1—HN1···S1^{i}	0.86 (2)	2.57 (3)	3.426 (7)	173 (10)
N2—HN2···I2^{ii}	0.85 (8)	3.02 (8)	3.657 (7)	133 (7)
C3—H3···I3^{iii}	0.95	3.12	4.035 (9)	163
C6—H6···I1^{iv}	0.95	3.14	3.927 (8)	142

Symmetry codes: (i) $-x+1, -y+3, -z+1$; (ii) $x-1, y+1, z$; (iii) $x, y+1, z$; (iv) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$.

Table 11
Hydrogen-bond geometry (Å, °) for (**MBZOX**)·(**1,2-F$_4$DIB**).

D—H···A	D—H	H···A	D···A	D—H···A
N1—HN1···S1^{i}	0.85 (8)	2.50 (8)	3.335 (6)	167 (8)
C3—H3···I2^{ii}	0.95	3.19	4.108 (7)	162

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

with **1,4-F$_4$DIB** were unsuccessful, suggesting the packing arrangement formed strictly by halogen bonding contains small but meaningful voids that must be occupied by the water molecule. Discrete hydrogen-bonded dimers are again observed by hydrogen bonding of the thioamides (Table 9). Differing from (**MMBZIM**)·(**1,2-F$_4$DIB**), with two halogen bonds to each S atom, 2(**MMBZIM**)·(**1,4-F4DIB**)·2(**H$_2$O**) utilizes one C—I···S halogen bond and one O—H···S hydrogen bond at each S atom. It is the halogen bonding that contributes to the formation of infinite chains by linking the discrete dimers. The water molecule also acts as an N—H···O hydrogen-bond acceptor from the N atom that does not participate in thioamide hydrogen bonding and so is an intermediate linker facilitating the formation of an expanded thioamide ribbon motif.

Finally, the combination of **1,3,5-F$_3$I$_3$B** and **MMBZIM** resulted in the cocrystal (**MMBZIM**)·(**1,3,5-F$_3$I$_3$B**), refined in the monoclinic space group $P2_1/c$ with one unique molecule of each component in the asymmetric unit. The overall packing motif in this structure is strikingly similar to that in (**MMBZIM**)·(**1,2-F$_4$DIB**). Two molecules of **MMBZIM** form dimeric pairs through hydrogen bonding of the thioamides (Table 10). The remaining N—H hydrogens are involved in weak N—H···I hydrogen bonds [H···I = 3.02 (8) Å]. A pair of C—I···S halogen bonds occurs at each S atom, contributing to chains propagating in the *a* direction. The third I atom is oriented as a potential acceptor for a C—F···I interaction, though the interaction distance is very near the sum of the van der Waals radii and it is unclear if there is a significant attraction to this interaction. Given the similar motifs of (**MMBZIM**)·(**1,3,5-F$_3$I$_3$B**) to (**MMBZIM**)·(**1,2-F$_4$DIB**), it may be that the C—F···I contact is merely coincident within the motif formed by the N—H···S and C—I···S interactions.

Table 12
Hydrogen-bond geometry (Å, °) for (**MBZOX**)·(**1,3-F$_4$DIB**).

D—H···A	D—H	H···A	D···A	D—H···A
N1—HN1···S1^{i}	0.88 (3)	2.52 (3)	3.3906 (19)	172 (3)
C3—H3···I1^{ii}	0.95	3.10	4.030 (2)	166

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

Table 13
Hydrogen-bond geometry (Å, °) for 2(**MBZOX**)·(**1,4-F$_4$DIB**).

D—H···A	D—H	H···A	D···A	D—H···A
N1—HN1···S1^{i}	0.87 (4)	2.45 (4)	3.316 (3)	178 (4)
C3—H3···I1^{ii}	0.95	3.16	4.066 (3)	159

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

3.4. Cocrystals of 2-mercaptobenzoxazole (MBZOX)

While infinite ribbons commonly formed through hydrogen bonding of the thioureas in **MBZIM**, substituting one secondary N atom for an O atom in 2-mercaptobenzoxazole (**MBZOX**) allows for the study of the structural motifs when only dimers can form through hydrogen bonding (Fig. 5). The structural literature surrounding **MBZOX** is sparse, limited to three reports of it acting as a ligand through the S atom in transition-metal complexes (McFarlane *et al.*, 1998; Nakahodo *et al.*, 2000; Mitra *et al.*, 2012) and its reaction with diiodine (Cristiani *et al.*, 1995). Combined with **1,2-F$_4$DIB**, the cocrystalline structure of (**MBZOX**)·(**1,2-F$_4$DIB**) was refined in the monoclinic space group $P2_1/n$, with one unique molecule each of **MBZOX** and **1,2-F$_4$DIB** in the asymmetric unit. Here, a hydrogen-bonding thioamide dimer is formed (Table 11), with each S atom acting as an acceptor to a single C—I···S halogen bond. The second I atom does not contribute to an additional halogen bond, instead being involved in a weak C—I···π interaction. This discrete four-molecule unit formed through hydrogen and halogen bonding stands in stark contrast to the infinite hydrogen-bonding ribbon with pendant halogen-bonded **1,2-F$_4$DIB** molecules observed in (**MBZIM**)·(**1,2-F$_4$DIB**). The pattern of interactions in (**MBZOX**)·(**1,3-F$_4$DIB**), which crystallizes in the monoclinic space group $P2_1/c$, with one molecule each of **MBZOX** and **1,3-F$_4$DIB** in the asymmetric unit, is more complex. Thioamide hydrogen-bonding dimers are once again observed (Table 12). These dimers stack along the *b* axis. Molecules of **1,3-F$_4$DIB** link neighboring stacks of dimers in the *a* direction. One of the I atoms serves as both a C—I···S halogen-bond donor and a C═S···I chalcogen-bond acceptor. The combination of halogen, chalcogen, and hydrogen-bonding results in the formation of a two-dimensional motif of intermolecular

Table 14
Hydrogen-bond geometry (Å, °) for (**MBZOX**)·(**1,3,5-F$_3$I$_3$B**).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—HN1···S1^{i}	0.85 (7)	2.53 (7)	3.377 (4)	176 (6)
C3—H3···I1^{ii}	0.95	3.04	3.969 (5)	167
C6—H6···I2^{iii}	0.95	3.23	4.009 (5)	140

Symmetry codes: (i) $-x+2, -y, -z+1$; (ii) $-x+2, -y+1, -z+1$; (iii) $x, -y+\frac{5}{2}, z-\frac{1}{2}$.

Table 15
Hydrogen-bond geometry (Å, °) for 3(**MBZTH**)·4(**1,2-F$_4$DIB**).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—HN2···S1	0.88	2.45	3.326 (14)	174
N1—HN1···S3	0.88	2.40	3.266 (14)	169
C6—H6···F10^{i}	0.95	2.60	3.29 (2)	130
N3—HN3···S5^{ii}	0.88	2.42	3.290 (14)	170
C17—H17···F16	0.95	2.30	3.232 (18)	166
C20—H20···F2	0.95	2.53	3.128 (18)	121
C20—H20···F3	0.95	2.54	3.181 (17)	125

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

interactions. In 2(**MBZOX**)·(**1,4-F$_4$DIB**), which was refined in the monoclinic space group *C*2/*c*, with one molecule of **MBZOX** and one-half of a molecule of **1,4-F$_4$DIB**, the packing motif is more reminiscent of its **MMBZIM** analogue. Thioamide hydrogen-bonding dimers are linked into chains through C—I···S halogen bonding (Table 13). The final example in the **MBZOX** series, (**MBZOX**)·(**1,3,5-F$_3$I$_3$B**), was refined in the monoclinic space group $P2_1/c$, with one molecule each of **MBZOX** and **1,3,5-F$_3$I$_3$B** in the asymmetric unit. Much of the packing is similar to (**MBZOX**)·(**1,3-F$_4$DIB**), with thioamide hydrogen-bonding dimers stacking in the *b* direction (Table 14). Neighboring stacks are linked along the *a* axis by both C—I···S halogen bonding and a C═S···I chalcogen bond to again form a two-dimensional substructure. In this instance though, the third I atom of **1,3,5-F$_3$I$_3$B** acts as a C—I···I halogen-bond donor, further consolidating the packing in the *c* direction to form a three-dimensional framework. In all cases of these **MBZOX** cocrystals, hydrogen- and halogen-bonding preference is given toward the thione S atom as the acceptor rather than the O atom of the heterocycle.

3.5. Cocrystals of 2-mercaptobenzothiazole (MBZTH)

As with **MBZOX**, 2-mercaptobenzothiazole lacks the thiourea functionality to allow for the formation of infinite ribbons through hydrogen bonding; however, the additional S atom can potentially act in either halogen- or chalcogen-bonding interactions (Fig. 6). Just as with **MBZOX**, the prior structural literature is dominated by examples of **MBZTH** acting as a ligand in transition-metal complexes (Aslanidis *et al.*, 2002; Zhou *et al.*, 2013*b*; Hadjikakou & Kubicki, 2000) or reactions with dihalides (Daga *et al.*, 2002; Koskinen *et al.*,

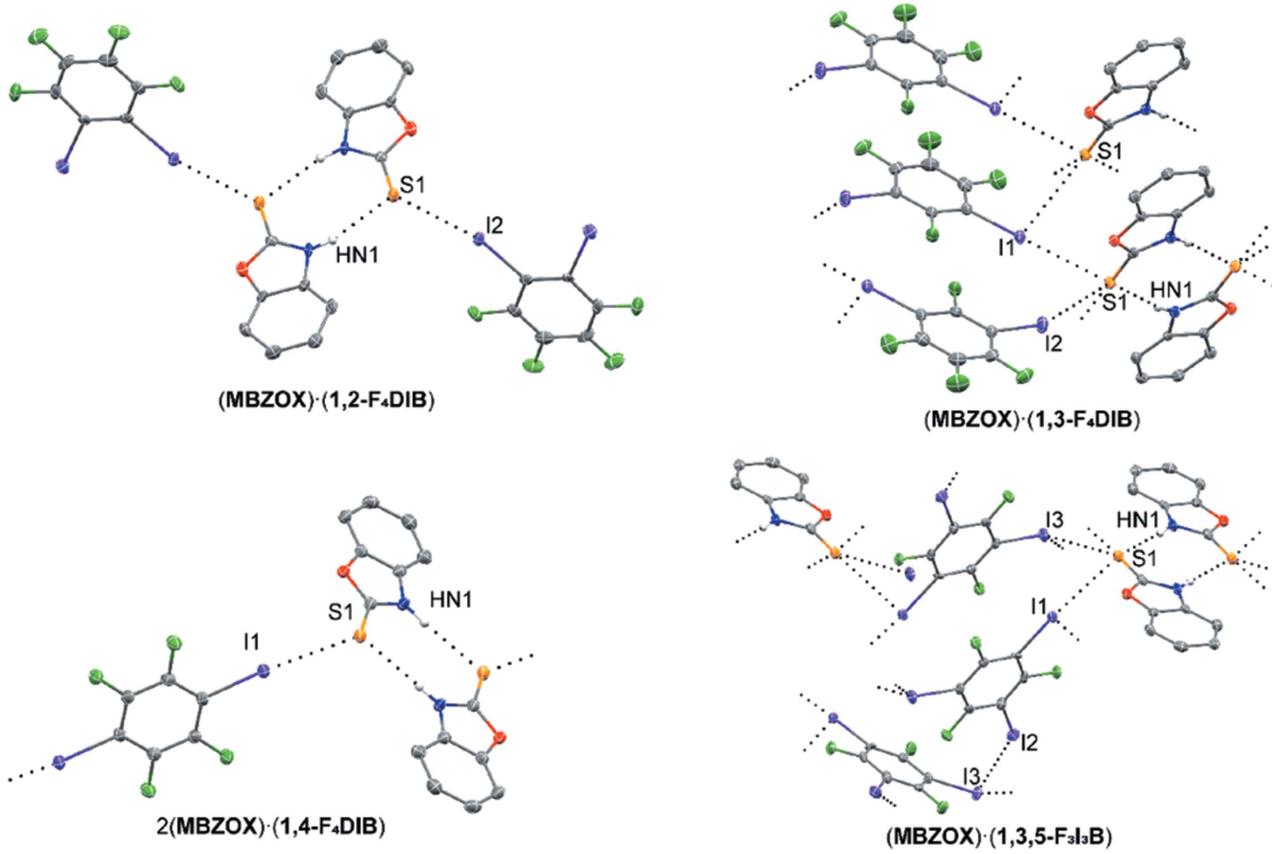


Figure 5
Cocrystalline structures containing **MBZOX**. Hydrogen and halogen bonding are indicated by black dotted lines. Displacement ellipsoids are drawn at the 50% probability level. H atoms, except those bound to N atoms, have been omitted for clarity.

2015*a*,*b*). The first and most complex of the **MBZTH** structures obtained, 3(**MBZTH**)·4(**1,2-F$_4$DIB**), crystallized in the triclinic space group $P\overline{1}$, with three molecules of **MBZTH** and four molecules of **1,2-F$_4$DIB** in the asymmetric unit. Thioamide dimers stack along the *a* axis (Table 15), with one molecule of **1,2-F$_4$DIB** within alternating layers. The remaining molecules of **1,2-F$_4$DIB** are oriented approximately perpendicular to the thioamide dimers, linking layers of the stack through a series of C—I···S halogen bonds. The intrastack molecule of **1,2-F$_4$DIB** is also linked to a molecule of **1,2-F$_4$DIB** on the edge of the stack through a C—I···I halogen bond. This complex series of interactions ultimately forms a three-dimensional framework.

The packing motif of (**MBZTH**)·(**1,3-F$_4$DIB**), refined in the triclinic space group $P\overline{1}$, with one molecule each of **MBZTH** and **1,3-F$_4$DIB** within the asymmetric unit, is similar to that of (**MMBZIM**)·(**1,2-F$_4$DIB**) and (**MMBZIM**)·(**1,3,5-F$_3$I$_3$B**). Thioamide hydrogen-bonding dimers (Table 16) are linked by a pair of unique C—I···S halogen bonds to the thione S atom, forming chains in the *c* direction. Crystallizing in the monoclinic

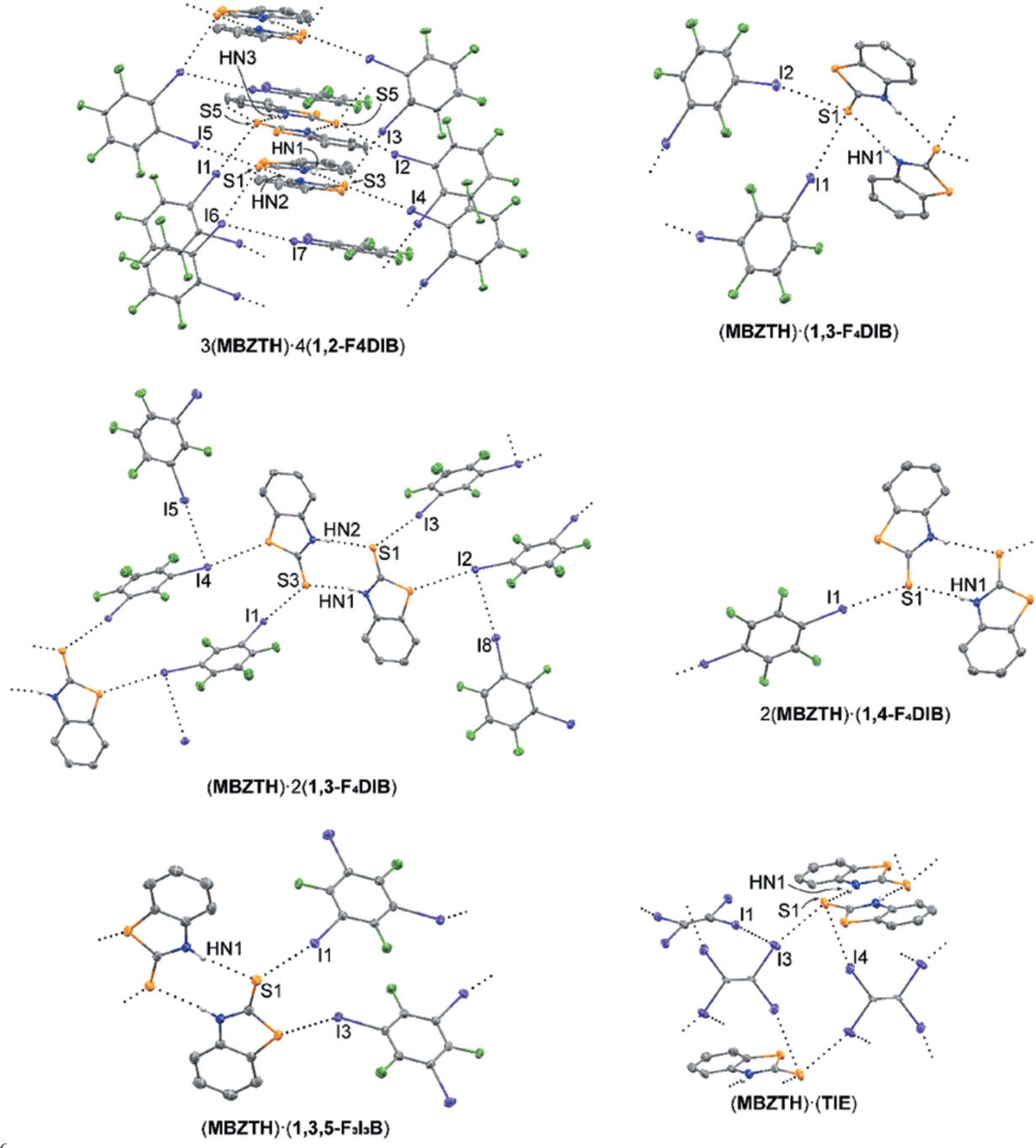


Figure 6
Cocrystalline structures containing **MBZTH**. Hydrogen and halogen bonding are indicated by black dotted lines. Displacement ellipsoids are drawn at the 50% probability level. H atoms, except those bound to N atoms, have been omitted for clarity.

Table 16
Hydrogen-bond geometry (Å, °) for (**MBZTH**)·(**1,3-F$_4$DIB**).

D—H···A	D—H	H···A	D···A	D—H···A
N1—HN1···S1^{i}	0.87 (3)	2.45 (3)	3.3120 (15)	175 (2)

Symmetry code: (i) $-x+2, -y+2, -z+2$.

Table 17
Hydrogen-bond geometry (Å, °) for (**MBZTH**)·2(**1,3-F$_4$DIB**).

D—H···A	D—H	H···A	D···A	D—H···A
N1—HN1···S3	0.89 (6)	2.51 (6)	3.376 (6)	165 (5)
C3—H3···I1	0.95	3.10	3.976 (7)	154
N2—HN2···S1	0.85 (3)	2.52 (3)	3.360 (6)	169 (7)
C10—H10···I3^{i}	0.95	3.09	4.006 (6)	161

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

Table 18
Hydrogen-bond geometry (Å, °) for 2(**MBZTH**)·(**1,4-F$_4$DIB**).

D—H···A	D—H	H···A	D···A	D—H···A
N1—HN1···S1^{i}	0.78 (3)	2.60 (3)	3.369 (2)	170 (3)
C3—H3···F1^{ii}	0.95	2.50	3.333 (3)	146
C6—H6···F2^{iii}	0.95	2.44	3.357 (3)	162

Symmetry codes: (i) $-x-1, -y+1, -z+1$; (ii) $-x, -y+1, -z+1$; (iii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.

space group $P2_1$, the asymmetric unit of (**MBZTH**)·2(**1,3-F$_4$DIB**) contains two unique molecules of **MBZTH** and four molecules of **1,3-F$_4$DIB**. In this case, the thioamide hydrogen-bonding dimers (Table 17) are linked by molecules of **1,3-F$_4$DIB** *via* C—I···S halogen bonding to form chains. These interactions occur to the thione and thiazole S atoms, with the interaction to the thione S atom occurring at a distance approximately 0.35 Å shorter than to the thiazole S atom. The remaining two molecules of **1,3-F$_4$DIB** are located as pendants along the chain, linked by C—I···I halogen bonding.

The packing motif of 2(**MBZTH**)·(**1,4-F$_4$DIB**), refined in the monoclinic space group $P2_1/n$, with one complete molecule of **MBZTH** and one-half of a molecule of **1,4-F$_4$DIB** in the asymmetric unit, is similar to that of 2(**MBZOX**)·(**1,4-F$_4$DIB**). Thioamide hydrogen-bonding dimers (Table 18) are linked into chains *via* C—I···S halogen bonding to the thione S atom. As the final example with an aromatic halogen-bond donor, (**MBZTH**)·(**1,3,5-F$_3$I$_3$B**) was obtained in the monoclinic space group $P2_1/c$, with one unique molecule each of both **MBZTH** and **1,3,5-F$_3$I$_3$B** in the asymmetric unit. The primary packing motif is similar to that of (**MBZTH**)·2(**1,3-F$_4$DIB**), with the thioamide hydrogen-bonding dimers (Table 19) linked into chains by C—I···S halogen bonds to both the thione and thiazole S atoms. The third I atom serves to link neighboring chains through a weak C—I···S—C interaction to a thiazole S atom; however, the geometry of this interaction [C—I···S = 149.3 (1) and 142.48 (13)°] is indicative of a dispersive Type I interaction and not a true halogen or chalcogen bond. Finally, (**MBZTH**)·(**TIE**) crystallized in the triclinic space group $P\overline{1}$ with one unique molecule of **MBZTH** and two unique half molecules of **TIE** in the asymmetric unit. Thioamide hydrogen-bonding dimers (Table 20) are linked into chains by C—I···S halogen bonding to the thione S atom. These chains are linked in the *ab* plane by additional C—I···S halogen bonding to the thione S atom. The second unique **TIE** molecule serves to consolidate the packing in the *c* direction *via* C—I···I halogen bonding, forming a three-dimensional framework.

Table 19
Hydrogen-bond geometry (Å, °) for (**MBZTH**)·(**1,3,5-F$_3$I$_3$B**).

D—H···A	D—H	H···A	D···A	D—H···A
N1—HN1···S1^{i}	0.86 (2)	2.54 (2)	3.389 (3)	172 (4)
C3—H3···I1^{ii}	0.95	3.03	3.928 (4)	159

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

Table 20
Hydrogen-bond geometry (Å, °) for (**MBZTH**)·(**TIE**).

D—H···A	D—H	H···A	D···A	D—H···A
N1—HN1···S1^{i}	0.85 (2)	2.43 (2)	3.275 (5)	170 (6)

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

4. Conclusion

A rich structural chemistry of cocrystals was observed between organoiodine molecules and heterocyclic thiones in the present study of 18 crystal structures. The structures are primarily directed by the co-operative effects of hydrogen- and halogen-bonding interactions. Certain features of the long-range structures were controlled through the selection of the heterocyclic thione, where the formation of primarily hydrogen-bonded ribbons in benzimidazoles could be truncated to hydrogen-bonded dimers in benzoxazoles and benzothiazoles. The hydrogen-bonded units were then aggregated into longer-range one- or two-dimensional motifs through C—I···S halogen bonding. Additional C—I···I halogen bonding, either through the stoichiometric excess of organoiodine or through the use of more iodine-rich organoiodine substrates (tetraiodoethylene, for example) extended some structures into three-dimensional frameworks. The R_{XB} value for the majority of the halogen-bonding interactions lies within a typical range from 0.85 to 1.0. The interactions to a thione S atom generally occurred at shorter distances than the thiane S atom, as expected due to the hybridization state. The linearity parameter, ψ, ranges from 0.02 to 0.83. This wide range is supported by the distribution of electron density on S or I acceptor atoms. Occasional C═S···I chalcogen bonding was observed. Halogen-bond preference toward the thione S atom over the heterocyclic O or S atom was observed in both the benzoxazoles and benzothiazoles. However, there were at least some occasional occurrences of C—I···S to the thiazole S atom.

References

Aakeroy, C. B., Bryce, D. L., Cavallo, G., Clark, T., Herrebout, W., Hill, J. G., Ho, P. S., Jentzsch, A. V., Legon, A. C., Matile, S., Metrangolo, P., Murray, J. S., Pilati, T., Politzer, P., Resnati, G.,

Spartz, C. L., Terraneo, G., Tew, D. P., Viger-Gravel, J. & Walker, N. R. (2015). In *Topics in Current Chemistry: Halogen Bonding I*. New York: Springer International Publishing.
Aakeroy, C. B., Bryce, D. L., Desiraju, G. R., Frontera, A., Legon, A. C., Nicotra, F., Rissanen, K., Scheiner, S., Terraneo, G., Metrangolo, P. & Resnati, G. (2019). *Pure Appl. Chem.* **91**, 1889–1892.
Achar, K. C. S., Hosamani, K. M. & Seetharamareddy, H. R. (2010). *Eur. J. Med. Chem.* **45**, 2048–2054.
Ajani, H., Carlsson, A. C. C., Cavallo, G., Deepa, P., Erdelyi, M., Fourmigue, M., Haukka, M., Hobza, P., Huber, S. M., Jin, W. J., Kolar, M. H., Lieffrig, J., Metrangolo, P., Pang, X., Pecina, A., Priimagi, A., Resnati, G., Rissanen, K., Saccone, M., Schindler, S., Taylor, M. S. & Veiga, A. X. (2015). In *Topics in Current Chemistry: Halogen Bonding II*. New York: Springer International Publishing.
Alasmary, F. A. S., Snelling, A. M., Zain, M. E., Alafeefy, A. M., Awaad, A. S. & Karodia, N. (2015). *Molecules*, **20**, 15206–15223.
Arman, H. D., Biella, S., Bruce, D. W., Fourmigue, M., Hanks, T. W., Karpfen, A., Kochi, J. K., Legon, A. C., Metrangolo, P., Pennington, W. T., Pilati, T., Resnati, G. & Rosokha, S. V. (2008). In *Structure and Bonding: Halogen Bonding*. New York: Springer International Publishing.
Arman, H. D., Gieseking, R. L., Hanks, T. W. & Pennington, W. T. (2010). *Chem. Commun.* **46**, 1854–1856.
Aslanidis, P., Cox, P. J., Karagiannidis, P., Hadjikakou, S. K. & Antoniadis, C. D. (2002). *Eur. J. Inorg. Chem.* **2002**, 2216–2222.
Auffinger, P., Hays, F. A., Westhof, E. & Ho, P. S. (2004). *Proc. Natl Acad. Sci. USA*, **101**, 16789–16794.
Banti, C. N., Kyros, L., Geromichalos, G. D., Kourkoumelis, N., Kubicki, M. & Hadjikakou, S. K. (2014). *Eur. J. Med. Chem.* **77**, 388–399.
Bruker (2017). *APEX3*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cavallo, G., Metrangolo, P., Milani, R., Pilati, T., Priimagi, A., Resnati, G. & Terraneo, G. (2016). *Chem. Rev.* **116**, 2478–2601.
Corradi, E., Meille, S. V., Messina, M. T., Metrangolo, P. & Resnati, G. (2000). *Angew. Chem. Int. Ed.* **39**, 1782–1786.
Cristiani, F., Devillanova, F. A., Isaia, F., Lippolis, V., Verani, G. & Demartin, F. (1995). *Polyhedron*, **14**, 2937–2943.
Daga, V., Hadjikakou, S. K., Hadjiliadis, N., Kubicki, M., Santos, J. & Butler, I. (2002). *Eur. J. Inorg. Chem.* **2002**, 1718–1728.
Desiraju, G. R., Ho, P. S., Kloo, L., Legon, A. C., Marquardt, R., Metrangolo, P., Politzer, P., Resnati, G. & Rissanen, K. (2013). *Pure Appl. Chem.* **85**, 1711–1713.
Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
Fletcher, S. R., McIver, E., Lewis, S., Burkamp, F., Leech, C., Mason, G., Boyce, S., Morrison, D., Richards, G., Sutton, K. & Jones, A. B. (2006). *Bioorg. Med. Chem. Lett.* **16**, 2872–2876.
Foks, H., Pancechowska-Ksepko, D., Kuzmierkiewicz, W., Zwolska, Z., Augustynowicz-Kopec, E. & Janowiec, M. (2006). *Chem. Heterocycl. Compd.* **42**, 611–614.
Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.
Hadjikakou, S. K. & Kubicki, M. (2000). *Polyhedron*, **19**, 2231–2236.
Happonen, L., Rautiainen, J. M. & Valkonen, A. (2021). *Cryst. Growth Des.* **21**, 3409–3419.
Koskinen, L., Hirva, P., Hasu, A., Jääskeläinen, S., Koivistoinen, J., Pettersson, M. & Haukka, M. (2015*a*). *CrystEngComm*, **17**, 2718–2727.
Koskinen, L., Jääskeläinen, S., Hirva, P. & Haukka, M. (2015*b*). *Cryst. Growth Des.* **15**, 1160–1167.
Legon, A. C. (1998). *Chem. Eur. J.* **4**, 1890–1897.
Lin, S., Cui, Y. Z., Qiu, Q. M., Han, H. L., Li, Z. F., Liu, M., Xin, X. L. & Jin, Q. H. (2017). *Polyhedron*, **134**, 319–329.
Macrae, C. F., Sovago, I., Cottrell, S. J., Galek, P. T. A., McCabe, P., Pidcock, E., Platings, M., Shields, G. P., Stevens, J. S., Towler, M. & Wood, P. A. (2020). *J. Appl. Cryst.* **53**, 226–235.
McFarlane, W., Akrivos, P. D., Aslanidis, P., Karagiannidis, P., Hatzisymeon, C., Numan, M. & Kokkou, S. (1998). *Inorg. Chim. Acta*, **281**, 121–125.
Metrangolo, P., Neukirch, H., Pilati, T. & Resnati, G. (2005). *Acc. Chem. Res.* **38**, 386–395.
Metrangolo, P. & Resnati, G. (2012). *Cryst. Growth Des.* **12**, 5835–5838.
Mitra, R., Das, S., Shinde, S. V., Sinha, S., Somasundaram, K. & Samuelson, A. G. (2012). *Chem. Eur. J.* **18**, 12278–12291.
Nakahodo, T., Horn, E. & Tiekink, E. R. T. (2000). *Acta Cryst.* C**56**, 1316–1318.
Ozturk, I. I., Hadjikakou, S. K., Hadjiliadis, N., Kourkoumelis, N., Kubicki, M., Tasiopoulos, A. J., Scleiman, H., Barsan, M. M., Butler, I. S. & Balzarini, J. (2009). *Inorg. Chem.* **48**, 2233–2245.
Parisini, E., Metrangolo, P., Pilati, T., Resnati, G. & Terraneo, G. (2011). *Chem. Soc. Rev.* **40**, 2267–2278.
Peloquin, A. J., Alapati, S., McMillen, C. D., Hanks, T. W. & Pennington, W. T. (2021*a*). *Molecules*, **26**, 4985–4994.
Peloquin, A. J., Hill, S. C., Arman, H. D., McMillen, C. D., Rabinovich, D. & Pennington, W. T. (2022). *J. Chem. Crystallogr.* **52**, 62–72.
Peloquin, A. J., McCollum, J. M., McMillen, C. D. & Pennington, W. T. (2021*b*). *Angew. Chem. Int. Ed.* **60**, 22983–22989.
Peloquin, A. J., McMillen, C. D., Iacono, S. T. & Pennington, W. T. (2021*c*). *Chem. Eur. J.* **27**, 8398–8405.
Peloquin, A. J., Ragusa, A. C., McMillen, C. D. & Pennington, W. T. (2021*d*). *Acta Cryst.* C**77**, 599–609.
Setter, C. J., Whittaker, J. J., Brock, A. J., Athukorala Arachchige, K. S., McMurtrie, J. C., Clegg, J. K. & Pfrunder, M. C. (2020). *CrystEngComm*, **22**, 1687–1690.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* C**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* A**71**, 3–8.
Zafar, M., Ramalakshmi, Rongala, Rongala, R., Pradhan, A. N., Pathak, K., Roisnel, T., Halet, J. F. & Ghosh, S. (2019). *Dalton Trans.* **48**, 7413–7424.
Zhou, P., Tian, F., Zou, J. & Shang, Z. (2010). *Mini Rev. Med. Chem.* **10**, 309–314.
Zhou, W. X., Yin, B., Li, J., Sun, W. J. & Zhang, F. X. (2013*a*). *Inorg. Chim. Acta*, **408**, 209–213.
Zhou, W. X., Yin, B., Li, J., Sun, W. J. & Zhang, F. X. (2013*b*). *Inorg. Chim. Acta*, **408**, 209–213.

supporting information

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Halogen, chalcogen, and hydrogen bonding in organoiodine cocrystals of heterocyclic thiones: imidazolidine-2-thione, 2-mercaptobenzimidazole, 2-mercapto-5-methylbenzimidazole, 2-mercaptobenzoxazole, and 2-mercaptobenzothiazole

Spencer Watts, Andrew J. Peloquin, Madhushi Bandara, Colin D. McMillen and William T. Pennington

Computing details

For all structures, data collection: *APEX3* (Bruker, 2017); cell refinement: *SAINT* (Bruker, 2017); data reduction: *SAINT* (Bruker, 2017); program(s) used to solve structure: SHELXT2018 (Sheldrick, 2015*a*); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015*b*). Molecular graphics: *Mercury* (Macrae *et al.*, 2020) for 2IT_13F4DIB, 4MBZIM_313F4DIB, MBZIM_14F4DIB, MBZIM_TIE, MMBZIM_12F4DIB, 2MMBZIM_14F4DIB_2H2O, MMBZIM_135F3I3B, MBZOX_12F4DIB, MBZOX_13F4DIB, 2MBZOX_14F4DIB, MBZOX_135F3I3B, 3MBZTH_412F4DIB, MBZTH_13F4DIB, MBZTH_213F4DIB, 2MBZTH_14F4DIB, MBZTH_135F3I3B, MBZTH_TIE; OLEX2 (Dolomanov *et al.*, 2009) for IT_135F3I3B. For all structures, software used to prepare material for publication: OLEX2 (Dolomanov *et al.*, 2009).

1,2,3,5-Tetrafluoro-4,6-diiodobenzene–imidazolidine-2-thione (1/2) (2IT_13F4DIB)

Crystal data

$C_6F_4I_2·2C_3H_6N_2S$
M_r = 606.18
Orthorhombic, *Pbcn*
a = 15.6704 (7) Å
b = 8.9924 (4) Å
c = 26.0573 (10) Å
V = 3671.9 (3) Å^3
Z = 8
$F(000)$ = 2288
D_x = 2.193 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9343 reflections
θ = 2.6–30.1°
μ = 3.69 mm^{-1}
T = 100 K
Block, colourless
0.18 × 0.17 × 0.13 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec IμS
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.639, T_{max} = 0.746
112821 measured reflections
5376 independent reflections
5198 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 30.1°, θ_{min} = 2.0°
h = −22→22
k = −12→12
l = −36→31

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.015$
$wR(F^2) = 0.032$
$S = 1.25$
5376 reflections
234 parameters
0 restraints
Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0054P)^2 + 3.3158P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 0.42$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ e Å^{-3}
Extinction correction: SHELXL2018 (Sheldrick, 2015*b*), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00082 (4)

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.71842 (2)	0.27502 (2)	0.20785 (2)	0.01326 (3)
I2	0.98485 (2)	0.54110 (2)	0.35028 (2)	0.01761 (3)
F1	0.89456 (6)	0.34626 (11)	0.26335 (4)	0.01975 (19)
F2	0.81145 (7)	0.69420 (11)	0.38910 (4)	0.0230 (2)
F3	0.64754 (6)	0.66108 (12)	0.36116 (4)	0.0232 (2)
F4	0.60595 (6)	0.48196 (12)	0.28175 (4)	0.0215 (2)
C7	0.74984 (10)	0.40891 (16)	0.27097 (5)	0.0139 (3)
C8	0.83358 (10)	0.42536 (17)	0.28725 (6)	0.0145 (3)
C9	0.85758 (10)	0.51990 (17)	0.32680 (6)	0.0157 (3)
C10	0.79313 (10)	0.59875 (17)	0.35087 (6)	0.0165 (3)
C11	0.70856 (10)	0.58350 (18)	0.33669 (6)	0.0172 (3)
C12	0.68786 (10)	0.49038 (18)	0.29640 (6)	0.0155 (3)
S1	0.68567 (2)	0.95036 (4)	0.61354 (2)	0.01476 (7)
N1	0.69251 (9)	0.72075 (15)	0.54616 (5)	0.0166 (3)
HN1	0.7189 (14)	0.672 (3)	0.5672 (9)	0.027 (6)*
N2	0.64832 (10)	0.92951 (15)	0.51306 (5)	0.0182 (3)
HN2	0.6289 (14)	1.015 (2)	0.5136 (8)	0.022 (5)*
C1	0.67475 (9)	0.86294 (17)	0.55568 (6)	0.0134 (3)
C2	0.68382 (11)	0.68448 (18)	0.49167 (6)	0.0186 (3)
H2A	0.644157	0.600134	0.486460	0.022*
H2B	0.739772	0.659716	0.476228	0.022*
C3	0.64743 (11)	0.82909 (18)	0.46895 (6)	0.0199 (3)
H3A	0.683895	0.867131	0.440842	0.024*
H3B	0.588726	0.814231	0.455882	0.024*
S2	0.42217 (3)	0.71986 (5)	0.49680 (2)	0.02184 (9)
N3	0.47631 (10)	0.51791 (16)	0.42741 (5)	0.0199 (3)
HN3	0.4952 (13)	0.467 (2)	0.4491 (9)	0.020 (5)*
N4	0.40214 (9)	0.69778 (16)	0.39417 (5)	0.0173 (3)

HN4	0.3816 (15)	0.783 (3)	0.3921 (9)	0.028 (6)*
C4	0.43369 (10)	0.64323 (17)	0.43758 (6)	0.0150 (3)
C5	0.46475 (10)	0.47080 (17)	0.37446 (6)	0.0166 (3)
H5A	0.423029	0.388469	0.371861	0.020*
H5B	0.519445	0.439328	0.358855	0.020*
C6	0.43059 (11)	0.61337 (18)	0.34929 (6)	0.0180 (3)
H6A	0.476022	0.666661	0.330344	0.022*
H6B	0.382641	0.591836	0.325695	0.022*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01584 (5)	0.01297 (5)	0.01098 (4)	−0.00009 (3)	−0.00092 (3)	0.00036 (3)
I2	0.01801 (5)	0.01630 (5)	0.01853 (5)	−0.00213 (4)	−0.00276 (4)	−0.00185 (4)
F1	0.0169 (4)	0.0213 (5)	0.0210 (5)	0.0041 (4)	0.0008 (4)	−0.0073 (4)
F2	0.0276 (5)	0.0234 (5)	0.0182 (5)	−0.0016 (4)	0.0000 (4)	−0.0098 (4)
F3	0.0216 (5)	0.0265 (5)	0.0215 (5)	0.0042 (4)	0.0058 (4)	−0.0079 (4)
F4	0.0143 (4)	0.0284 (5)	0.0217 (5)	0.0006 (4)	0.0006 (4)	−0.0042 (4)
C7	0.0190 (7)	0.0121 (6)	0.0105 (6)	−0.0010 (5)	0.0006 (5)	0.0002 (5)
C8	0.0170 (7)	0.0124 (6)	0.0141 (6)	0.0019 (5)	0.0012 (5)	−0.0001 (5)
C9	0.0175 (7)	0.0140 (7)	0.0155 (7)	−0.0009 (5)	−0.0013 (5)	0.0000 (5)
C10	0.0222 (8)	0.0144 (7)	0.0128 (6)	−0.0015 (6)	0.0005 (6)	−0.0015 (5)
C11	0.0205 (7)	0.0159 (7)	0.0152 (7)	0.0022 (6)	0.0043 (6)	−0.0010 (6)
C12	0.0150 (7)	0.0167 (7)	0.0146 (6)	−0.0010 (6)	0.0007 (5)	0.0014 (5)
S1	0.01883 (17)	0.01408 (16)	0.01138 (15)	0.00309 (13)	−0.00079 (13)	0.00015 (13)
N1	0.0220 (7)	0.0127 (6)	0.0150 (6)	0.0032 (5)	−0.0018 (5)	0.0014 (5)
N2	0.0277 (7)	0.0133 (6)	0.0136 (6)	0.0055 (5)	−0.0030 (5)	−0.0008 (5)
C1	0.0119 (6)	0.0140 (6)	0.0142 (6)	0.0004 (5)	0.0011 (5)	0.0008 (5)
C2	0.0259 (8)	0.0148 (7)	0.0152 (7)	0.0014 (6)	0.0001 (6)	−0.0028 (6)
C3	0.0276 (8)	0.0180 (7)	0.0141 (7)	0.0030 (6)	−0.0023 (6)	−0.0026 (6)
S2	0.0339 (2)	0.01651 (18)	0.01508 (17)	0.01055 (16)	−0.00313 (16)	−0.00093 (14)
N3	0.0280 (7)	0.0164 (6)	0.0151 (6)	0.0094 (6)	−0.0051 (5)	0.0000 (5)
N4	0.0212 (7)	0.0146 (6)	0.0161 (6)	0.0054 (5)	−0.0028 (5)	0.0010 (5)
C4	0.0143 (7)	0.0127 (6)	0.0179 (7)	0.0004 (5)	−0.0011 (5)	0.0015 (5)
C5	0.0197 (7)	0.0139 (7)	0.0161 (7)	0.0018 (6)	0.0003 (6)	−0.0003 (5)
C6	0.0221 (8)	0.0167 (7)	0.0153 (7)	0.0043 (6)	−0.0022 (6)	0.0002 (6)

Geometric parameters (Å, º)

I1—C7	2.0969 (14)	N2—C3	1.462 (2)
I2—C9	2.0947 (16)	C2—H2A	0.9900
F1—C8	1.3442 (17)	C2—H2B	0.9900
F2—C10	1.3459 (17)	C2—C3	1.538 (2)
F3—C11	1.3445 (18)	C3—H3A	0.9900
F4—C12	1.3412 (18)	C3—H3B	0.9900
C7—C8	1.387 (2)	S2—C4	1.6995 (16)
C7—C12	1.385 (2)	N3—HN3	0.79 (2)
C8—C9	1.388 (2)	N3—C4	1.337 (2)

C9—C10	1.384 (2)	N3—C5	1.455 (2)
C10—C11	1.383 (2)	N4—HN4	0.83 (2)
C11—C12	1.382 (2)	N4—C4	1.328 (2)
S1—C1	1.7088 (15)	N4—C6	1.464 (2)
N1—HN1	0.81 (2)	C5—H5A	0.9900
N1—C1	1.332 (2)	C5—H5B	0.9900
N1—C2	1.463 (2)	C5—C6	1.536 (2)
N2—HN2	0.83 (2)	C6—H6A	0.9900
N2—C1	1.3280 (19)	C6—H6B	0.9900

C8—C7—I1	121.56 (11)	H2A—C2—H2B	109.1
C12—C7—I1	120.94 (11)	C3—C2—H2A	111.2
C12—C7—C8	117.43 (14)	C3—C2—H2B	111.2
F1—C8—C7	118.31 (13)	N2—C3—C2	102.49 (12)
F1—C8—C9	118.39 (14)	N2—C3—H3A	111.3
C7—C8—C9	123.29 (14)	N2—C3—H3B	111.3
C8—C9—I2	122.05 (11)	C2—C3—H3A	111.3
C10—C9—I2	121.04 (11)	C2—C3—H3B	111.3
C10—C9—C8	116.90 (14)	H3A—C3—H3B	109.2
F2—C10—C9	120.43 (14)	C4—N3—HN3	122.5 (16)
F2—C10—C11	117.74 (14)	C4—N3—C5	111.80 (13)
C11—C10—C9	121.83 (14)	C5—N3—HN3	124.0 (16)
F3—C11—C10	120.23 (14)	C4—N4—HN4	122.7 (16)
F3—C11—C12	120.52 (15)	C4—N4—C6	112.06 (13)
C12—C11—C10	119.23 (14)	C6—N4—HN4	122.8 (16)
F4—C12—C7	120.34 (14)	N3—C4—S2	125.10 (12)
F4—C12—C11	118.37 (14)	N4—C4—S2	125.73 (12)
C11—C12—C7	121.29 (15)	N4—C4—N3	109.17 (14)
C1—N1—HN1	119.7 (16)	N3—C5—H5A	111.4
C1—N1—C2	112.04 (13)	N3—C5—H5B	111.4
C2—N1—HN1	125.6 (16)	N3—C5—C6	101.85 (12)
C1—N2—HN2	121.3 (15)	H5A—C5—H5B	109.3
C1—N2—C3	112.46 (13)	C6—C5—H5A	111.4
C3—N2—HN2	125.8 (15)	C6—C5—H5B	111.4
N1—C1—S1	125.81 (12)	N4—C6—C5	101.41 (12)
N2—C1—S1	124.18 (12)	N4—C6—H6A	111.5
N2—C1—N1	110.01 (14)	N4—C6—H6B	111.5
N1—C2—H2A	111.2	C5—C6—H6A	111.5
N1—C2—H2B	111.2	C5—C6—H6B	111.5
N1—C2—C3	102.68 (12)	H6A—C6—H6B	109.3

I1—C7—C8—F1	−3.75 (19)	C9—C10—C11—C12	−1.9 (2)
I1—C7—C8—C9	175.92 (12)	C10—C11—C12—F4	−177.15 (14)
I1—C7—C12—F4	1.7 (2)	C10—C11—C12—C7	1.9 (2)
I1—C7—C12—C11	−177.34 (12)	C12—C7—C8—F1	179.43 (13)
I2—C9—C10—F2	1.9 (2)	C12—C7—C8—C9	−0.9 (2)
I2—C9—C10—C11	−178.45 (12)	N1—C2—C3—N2	4.94 (17)
F1—C8—C9—I2	−0.4 (2)	C1—N1—C2—C3	−5.82 (18)

F1—C8—C9—C10	−179.48 (14)	C1—N2—C3—C2	−2.96 (19)
F2—C10—C11—F3	−0.8 (2)	C2—N1—C1—S1	−174.62 (12)
F2—C10—C11—C12	177.76 (14)	C2—N1—C1—N2	4.27 (19)
F3—C11—C12—F4	1.4 (2)	C3—N2—C1—S1	178.31 (12)
F3—C11—C12—C7	−179.58 (14)	C3—N2—C1—N1	−0.6 (2)
C7—C8—C9—I2	179.89 (11)	N3—C5—C6—N4	−18.18 (16)
C7—C8—C9—C10	0.9 (2)	C4—N3—C5—C6	16.94 (18)
C8—C7—C12—F4	178.51 (14)	C4—N4—C6—C5	15.47 (18)
C8—C7—C12—C11	−0.5 (2)	C5—N3—C4—S2	172.13 (12)
C8—C9—C10—F2	−179.09 (14)	C5—N3—C4—N4	−7.96 (19)
C8—C9—C10—C11	0.6 (2)	C6—N4—C4—S2	174.32 (12)
C9—C10—C11—F3	179.53 (14)	C6—N4—C4—N3	−5.59 (19)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···S1^{i}	0.81 (2)	2.77 (2)	3.5551 (14)	163 (2)
N2—H*N*2···S2^{ii}	0.83 (2)	2.53 (2)	3.3507 (14)	172 (2)
C2—H2*B*···F2	0.99	2.55	3.3392 (19)	136
C3—H3*B*···S2	0.99	2.94	3.7351 (19)	138
N3—H*N*3···S2^{iii}	0.79 (2)	2.54 (2)	3.3171 (15)	167 (2)
N4—H*N*4···I2^{iv}	0.83 (2)	3.31 (2)	3.7383 (14)	114.9 (18)
N4—H*N*4···S1^{ii}	0.83 (2)	2.63 (2)	3.4562 (14)	179 (2)
C5—H5*A*···I1^{v}	0.99	3.20	3.9922 (16)	138
C5—H5*B*···F4	0.99	2.45	3.2774 (19)	140
C6—H6*B*···I1^{vi}	0.99	3.18	3.9223 (16)	133

Symmetry codes: (i) −*x*+3/2, *y*−1/2, *z*; (ii) −*x*+1, −*y*+2, −*z*+1; (iii) −*x*+1, −*y*+1, −*z*+1; (iv) −*x*+3/2, *y*+1/2, *z*; (v) −*x*+1, *y*, −*z*+1/2; (vi) *x*−1/2, *y*+1/2, −*z*+1/2.

Imidazolidine-2-thione–1,3,5-trifluoro-2,4,6-triiodobenzene (1/1) (IT_135F3I3B)

Crystal data

$C_6F_3I_3·C_3H_6N_2S$
M_r = 611.92
Orthorhombic, *Pbca*
a = 18.0407 (14) Å
b = 7.2816 (6) Å
c = 22.1250 (19) Å
V = 2906.5 (4) Å^3
Z = 8
F(000) = 2208
D_x = 2.797 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 9914 reflections
θ = 2.9–28.3°
μ = 6.61 mm^{-1}
T = 100 K
Tabular, colourless
0.22 × 0.08 × 0.04 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec I*μ*S
φ and *ω* scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.563, T_{max} = 0.746
49179 measured reflections
3615 independent reflections
3220 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 28.3°, θ_{min} = 2.2°
h = −24→24
k = −9→9
l = −28→29

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.019$
$wR(F^2) = 0.040$
$S = 1.11$
3615 reflections
172 parameters
2 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0114P)^2 + 5.9439P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.57$ e Å^{-3}
$\Delta\rho_{min} = -0.77$ e Å^{-3}
Extinction correction: SHELXL2018 (Sheldrick, 2015*b*), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.000108 (15)

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.53750 (2)	0.23369 (3)	0.54191 (2)	0.01895 (5)
I2	0.82382 (2)	0.16514 (2)	0.68496 (2)	0.01507 (5)
I3	0.83267 (2)	0.32805 (2)	0.41594 (2)	0.01451 (5)
F1	0.65074 (9)	0.1654 (2)	0.64879 (8)	0.0189 (4)
F2	0.88045 (8)	0.2474 (2)	0.55242 (8)	0.0197 (4)
F3	0.65981 (9)	0.3180 (2)	0.44277 (8)	0.0179 (3)
C4	0.65271 (14)	0.2418 (4)	0.54544 (13)	0.0139 (5)
C5	0.69034 (15)	0.2057 (4)	0.59879 (13)	0.0146 (5)
C6	0.76726 (14)	0.2079 (4)	0.60287 (13)	0.0135 (5)
C7	0.80537 (14)	0.2449 (4)	0.54993 (13)	0.0140 (5)
C8	0.77196 (14)	0.2814 (4)	0.49545 (13)	0.0133 (5)
C9	0.69470 (14)	0.2803 (4)	0.49494 (13)	0.0137 (5)
S1	0.57097 (4)	0.61400 (10)	0.79736 (3)	0.01671 (14)
N1	0.52694 (14)	0.2877 (4)	0.84174 (13)	0.0228 (6)
HN1	0.4953 (19)	0.345 (6)	0.8617 (18)	0.057 (14)*
N2	0.62179 (16)	0.2684 (4)	0.78288 (13)	0.0257 (6)
HN2	0.6527 (16)	0.308 (5)	0.7585 (14)	0.029 (10)*
C1	0.57324 (15)	0.3832 (4)	0.80740 (12)	0.0161 (6)
C2	0.54227 (16)	0.0908 (4)	0.84203 (14)	0.0222 (6)
H2A	0.498578	0.019283	0.828618	0.027*
H2B	0.557562	0.048198	0.882651	0.027*
C3	0.60613 (19)	0.0758 (4)	0.79654 (16)	0.0277 (7)
H3A	0.649751	0.014419	0.814660	0.033*
H3B	0.590783	0.007958	0.759844	0.033*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01058 (8)	0.02130 (10)	0.02496 (11)	0.00013 (7)	0.00038 (7)	−0.00336 (8)
I2	0.01700 (9)	0.01397 (9)	0.01424 (10)	−0.00039 (6)	−0.00190 (7)	0.00115 (7)
I3	0.01480 (8)	0.01468 (9)	0.01405 (9)	0.00001 (6)	0.00204 (7)	0.00044 (7)
F1	0.0176 (8)	0.0235 (9)	0.0157 (9)	−0.0029 (7)	0.0045 (7)	0.0016 (7)
F2	0.0101 (7)	0.0284 (10)	0.0205 (9)	−0.0005 (6)	−0.0003 (6)	0.0023 (8)
F3	0.0170 (7)	0.0204 (9)	0.0163 (9)	0.0018 (7)	−0.0034 (6)	0.0024 (7)
C4	0.0098 (11)	0.0127 (13)	0.0193 (14)	−0.0006 (10)	−0.0004 (10)	−0.0018 (11)
C5	0.0172 (12)	0.0111 (13)	0.0155 (14)	−0.0027 (10)	0.0038 (11)	−0.0007 (11)
C6	0.0161 (12)	0.0118 (13)	0.0124 (13)	0.0014 (10)	−0.0043 (10)	−0.0012 (10)
C7	0.0118 (11)	0.0110 (13)	0.0191 (15)	0.0014 (10)	−0.0010 (10)	0.0000 (11)
C8	0.0141 (12)	0.0111 (13)	0.0148 (14)	0.0003 (10)	0.0033 (10)	−0.0016 (11)
C9	0.0137 (12)	0.0120 (13)	0.0153 (14)	0.0024 (10)	−0.0036 (10)	−0.0001 (11)
S1	0.0211 (3)	0.0144 (3)	0.0146 (3)	0.0003 (3)	0.0002 (3)	0.0002 (3)
N1	0.0236 (13)	0.0181 (13)	0.0267 (15)	−0.0027 (10)	0.0051 (11)	0.0020 (11)
N2	0.0321 (14)	0.0158 (13)	0.0292 (16)	0.0020 (11)	0.0127 (12)	0.0046 (12)
C1	0.0168 (13)	0.0223 (15)	0.0092 (14)	−0.0006 (11)	−0.0037 (10)	−0.0001 (11)
C2	0.0244 (14)	0.0209 (15)	0.0213 (16)	−0.0062 (12)	−0.0049 (12)	0.0046 (13)
C3	0.0397 (18)	0.0155 (15)	0.0278 (18)	0.0006 (14)	0.0044 (15)	0.0037 (13)

Geometric parameters (Å, º)

I1—C4	2.081 (2)	S1—C1	1.696 (3)
I2—C6	2.106 (3)	N1—HN1	0.831 (19)
I3—C8	2.100 (3)	N1—C1	1.326 (4)
F1—C5	1.349 (3)	N1—C2	1.460 (4)
F2—C7	1.356 (3)	N2—HN2	0.827 (18)
F3—C9	1.343 (3)	N2—C1	1.327 (4)
C4—C5	1.387 (4)	N2—C3	1.462 (4)
C4—C9	1.379 (4)	C2—H2A	0.9900
C5—C6	1.391 (4)	C2—H2B	0.9900
C6—C7	1.385 (4)	C2—C3	1.534 (4)
C7—C8	1.374 (4)	C3—H3A	0.9900
C8—C9	1.394 (4)	C3—H3B	0.9900
C5—C4—I1	121.0 (2)	C2—N1—HN1	128 (3)
C9—C4—I1	121.6 (2)	C1—N2—HN2	119 (3)
C9—C4—C5	117.4 (2)	C1—N2—C3	113.1 (3)
F1—C5—C4	118.7 (2)	C3—N2—HN2	127 (3)
F1—C5—C6	118.5 (3)	N1—C1—S1	125.4 (2)
C4—C5—C6	122.8 (3)	N1—C1—N2	108.7 (3)
C5—C6—I2	122.5 (2)	N2—C1—S1	125.9 (2)
C7—C6—I2	121.18 (19)	N1—C2—H2A	111.4
C7—C6—C5	116.3 (2)	N1—C2—H2B	111.4
F2—C7—C6	117.7 (2)	N1—C2—C3	102.1 (2)
F2—C7—C8	118.1 (2)	H2A—C2—H2B	109.2

C8—C7—C6	124.2 (2)	C3—C2—H2A	111.4
C7—C8—I3	122.51 (19)	C3—C2—H2B	111.4
C7—C8—C9	116.4 (3)	N2—C3—C2	102.3 (3)
C9—C8—I3	121.0 (2)	N2—C3—H3A	111.3
F3—C9—C4	118.7 (2)	N2—C3—H3B	111.3
F3—C9—C8	118.3 (2)	C2—C3—H3A	111.3
C4—C9—C8	122.9 (3)	C2—C3—H3B	111.3
C1—N1—HN1	118 (3)	H3A—C3—H3B	109.2
C1—N1—C2	113.5 (3)		

I1—C4—C5—F1	−0.2 (3)	C5—C6—C7—F2	−179.8 (2)
I1—C4—C5—C6	179.3 (2)	C5—C6—C7—C8	1.1 (4)
I1—C4—C9—F3	1.7 (4)	C6—C7—C8—I3	−177.9 (2)
I1—C4—C9—C8	−178.1 (2)	C6—C7—C8—C9	0.1 (4)
I2—C6—C7—F2	1.9 (3)	C7—C8—C9—F3	179.0 (2)
I2—C6—C7—C8	−177.3 (2)	C7—C8—C9—C4	−1.2 (4)
I3—C8—C9—F3	−2.9 (3)	C9—C4—C5—F1	−179.2 (2)
I3—C8—C9—C4	176.8 (2)	C9—C4—C5—C6	0.2 (4)
F1—C5—C6—I2	−3.4 (4)	N1—C2—C3—N2	5.8 (3)
F1—C5—C6—C7	178.2 (2)	C1—N1—C2—C3	−3.7 (3)
F2—C7—C8—I3	2.9 (4)	C1—N2—C3—C2	−6.8 (4)
F2—C7—C8—C9	−179.1 (2)	C2—N1—C1—S1	−179.8 (2)
C4—C5—C6—I2	177.1 (2)	C2—N1—C1—N2	−0.4 (4)
C4—C5—C6—C7	−1.2 (4)	C3—N2—C1—S1	−175.8 (2)
C5—C4—C9—F3	−179.2 (2)	C3—N2—C1—N1	4.8 (4)
C5—C4—C9—C8	1.0 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H*N*2···I2^{i}	0.83 (2)	3.10 (3)	3.742 (3)	137 (3)
C2—H2*B*···I1^{ii}	0.99	3.31	3.927 (3)	122
C2—H2*B*···F3^{iii}	0.99	2.47	3.147 (3)	125

Symmetry codes: (i) −*x*+3/2, *y*+1/2, *z*; (ii) −*x*+1, *y*−1/2, −*z*+3/2; (iii) *x*, −*y*+1/2, *z*+1/2.

1*H*-1,3-Benzodiazole-2-thiol–1,2,3,5-tetrafluoro-4,6-diiodobenzene (4/3) (4MBZIM_313F4DIB)

Crystal data

$3C_6F_4I_2·4C_7H_6N_2S$
M_r = 1806.37
Triclinic, $P\overline{1}$
a = 8.4573 (14) Å
b = 17.725 (3) Å
c = 18.759 (4) Å
α = 106.997 (7)°
β = 93.229 (7)°
γ = 92.034 (7)°
V = 2680.9 (9) Å^3

Z = 2
F(000) = 1692
D_x = 2.238 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 9879 reflections
θ = 2.4–27.5°
μ = 3.72 mm^{-1}
T = 100 K
Needle, colourless
0.34 × 0.04 × 0.04 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec IμS
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.668, T_{max} = 0.746
118524 measured reflections
12297 independent reflections
10558 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 27.6°, θ_{min} = 2.2°
h = −10→10
k = −23→23
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.041
S = 1.06
12297 reflections
717 parameters
8 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0068P)^2 + 2.3276P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.75 e Å^{-3}

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.

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

	x	y	z	U_{iso}*/U_{eq}
I1	0.23723 (2)	0.28696 (2)	0.64287 (2)	0.01892 (4)
I2	0.11203 (2)	0.62311 (2)	0.81696 (2)	0.02185 (4)
F29	0.12514 (17)	0.43584 (9)	0.76730 (8)	0.0228 (3)
F30	0.28968 (19)	0.64658 (9)	0.67800 (9)	0.0259 (3)
F31	0.41295 (19)	0.54429 (9)	0.56177 (9)	0.0271 (4)
F32	0.38986 (17)	0.38762 (9)	0.54469 (8)	0.0234 (3)
C29	0.2585 (3)	0.40830 (15)	0.65651 (14)	0.0161 (5)
C30	0.1965 (3)	0.46280 (16)	0.71636 (14)	0.0182 (5)
C31	0.2045 (3)	0.54314 (15)	0.72577 (14)	0.0166 (5)
C32	0.2787 (3)	0.56938 (15)	0.67263 (14)	0.0186 (5)
C33	0.3417 (3)	0.51713 (16)	0.61237 (14)	0.0193 (5)
C34	0.3307 (3)	0.43733 (16)	0.60458 (14)	0.0183 (5)
I3	0.39366 (2)	0.29864 (2)	0.15711 (2)	0.02594 (4)
I4	0.19057 (2)	0.58106 (2)	0.39910 (2)	0.02628 (4)
F33	0.31982 (19)	0.47479 (9)	0.24734 (9)	0.0278 (4)
F34	0.11956 (18)	0.43808 (10)	0.46524 (9)	0.0290 (4)
F35	0.17740 (18)	0.28360 (10)	0.41706 (9)	0.0295 (4)
F36	0.30202 (17)	0.22313 (9)	0.28451 (9)	0.0256 (3)
C35	0.2209 (3)	0.46038 (15)	0.35750 (15)	0.0190 (5)
C36	0.2842 (3)	0.42746 (16)	0.28917 (14)	0.0191 (5)
C37	0.3114 (3)	0.34781 (15)	0.26241 (14)	0.0178 (5)

C38	0.2759 (3)	0.30052 (15)	0.30711 (15)	0.0192 (5)
C39	0.2115 (3)	0.33102 (16)	0.37517 (15)	0.0210 (6)
C40	0.1836 (3)	0.40999 (16)	0.39927 (14)	0.0200 (5)
I5	0.82526 (2)	0.39902 (2)	−0.11345 (2)	0.02532 (4)
I6	0.75419 (2)	0.73973 (2)	0.07191 (2)	0.01718 (4)
F37	0.85766 (18)	0.58847 (9)	−0.05559 (8)	0.0244 (3)
F38	0.59562 (17)	0.64129 (9)	0.16783 (8)	0.0218 (3)
F39	0.54190 (18)	0.48581 (9)	0.14581 (9)	0.0262 (4)
F40	0.63996 (18)	0.38040 (9)	0.02360 (9)	0.0255 (3)
C41	0.7536 (3)	0.48240 (15)	−0.01841 (14)	0.0169 (5)
C42	0.7782 (3)	0.56261 (15)	−0.00623 (14)	0.0164 (5)
C43	0.7249 (3)	0.61822 (14)	0.05532 (14)	0.0149 (5)
C44	0.6468 (3)	0.59054 (15)	0.10618 (14)	0.0168 (5)
C45	0.6198 (3)	0.51085 (15)	0.09575 (14)	0.0180 (5)
C46	0.6721 (3)	0.45764 (15)	0.03328 (15)	0.0182 (5)
S1	1.26980 (7)	0.02971 (4)	0.13364 (4)	0.01658 (13)
N1	1.3937 (2)	−0.08314 (13)	0.19002 (11)	0.0155 (4)
HN1	1.487 (2)	−0.0747 (18)	0.1788 (17)	0.031 (9)*
N2	1.1363 (2)	−0.08180 (12)	0.18912 (11)	0.0153 (4)
HN2	1.041 (2)	−0.0708 (15)	0.1806 (14)	0.015 (7)*
C1	1.2668 (3)	−0.04645 (15)	0.17100 (13)	0.0158 (5)
C2	1.3451 (3)	−0.14290 (15)	0.21949 (13)	0.0154 (5)
C3	1.4285 (3)	−0.19430 (15)	0.24861 (14)	0.0188 (5)
H3	1.540814	−0.194912	0.248974	0.023*
C4	1.3406 (3)	−0.24474 (16)	0.27716 (14)	0.0208 (6)
H4	1.393923	−0.280671	0.297743	0.025*
C5	1.1748 (3)	−0.24408 (16)	0.27645 (14)	0.0197 (5)
H5	1.118578	−0.279849	0.296263	0.024*
C6	1.0905 (3)	−0.19247 (15)	0.24751 (14)	0.0182 (5)
H6	0.978144	−0.191915	0.247143	0.022*
C7	1.1792 (3)	−0.14174 (15)	0.21913 (13)	0.0159 (5)
S2	0.76230 (7)	−0.07080 (4)	0.13517 (3)	0.01460 (12)
N3	0.8902 (2)	0.04164 (12)	0.07893 (12)	0.0142 (4)
HN3	0.985 (2)	0.0339 (17)	0.0913 (16)	0.026 (8)*
N4	0.6315 (2)	0.03610 (12)	0.07390 (11)	0.0134 (4)
HN4	0.539 (2)	0.0257 (15)	0.0851 (15)	0.016 (7)*
C8	0.7619 (3)	0.00336 (14)	0.09496 (13)	0.0135 (5)
C9	0.8425 (3)	0.10176 (14)	0.04983 (13)	0.0149 (5)
C10	0.9275 (3)	0.15703 (15)	0.02577 (14)	0.0186 (5)
H10	1.040174	0.160378	0.028830	0.022*
C11	0.8386 (3)	0.20721 (15)	−0.00307 (15)	0.0199 (5)
H11	0.892259	0.246317	−0.019649	0.024*
C12	0.6733 (3)	0.20197 (15)	−0.00842 (14)	0.0185 (5)
H12	0.617475	0.236637	−0.029681	0.022*
C13	0.5882 (3)	0.14726 (15)	0.01657 (13)	0.0160 (5)
H13	0.475508	0.143780	0.013282	0.019*
C14	0.6767 (3)	0.09798 (14)	0.04661 (13)	0.0137 (5)
S3	0.21077 (7)	1.09011 (4)	0.59658 (4)	0.01674 (13)

N5	0.3335 (2)	0.98621 (12)	0.66496 (12)	0.0153 (4)
HN5	0.427 (2)	0.9957 (18)	0.6541 (17)	0.035 (9)*
N6	0.0755 (2)	0.98679 (12)	0.66091 (12)	0.0149 (4)
HN6	−0.020 (2)	0.9958 (16)	0.6501 (15)	0.021 (8)*
C15	0.2063 (3)	1.02032 (14)	0.64225 (13)	0.0147 (5)
C16	0.2825 (3)	0.92908 (14)	0.69697 (13)	0.0149 (5)
C17	0.3645 (3)	0.87884 (15)	0.72898 (14)	0.0196 (5)
H17	0.477019	0.878891	0.731657	0.024*
C18	0.2730 (3)	0.82880 (15)	0.75670 (14)	0.0211 (6)
H18	0.324318	0.793463	0.778775	0.025*
C19	0.1078 (3)	0.82884 (15)	0.75312 (14)	0.0213 (6)
H19	0.049812	0.793080	0.772293	0.026*
C20	0.0256 (3)	0.87954 (15)	0.72240 (14)	0.0186 (5)
H20	−0.086842	0.880244	0.720810	0.022*
C21	0.1171 (3)	0.92909 (14)	0.69418 (13)	0.0141 (5)
S4	−0.29930 (7)	0.99445 (4)	0.61172 (3)	0.01608 (12)
N7	−0.1672 (2)	1.09905 (13)	0.54729 (12)	0.0157 (4)
HN7	−0.073 (2)	1.0901 (18)	0.5580 (17)	0.033 (9)*
N8	−0.4249 (2)	1.09692 (13)	0.54319 (12)	0.0156 (4)
HN8	−0.519 (2)	1.0848 (17)	0.5511 (17)	0.029 (8)*
C22	−0.2972 (3)	1.06481 (14)	0.56708 (13)	0.0146 (5)
C23	−0.2121 (3)	1.15416 (14)	0.51139 (13)	0.0145 (5)
C24	−0.1251 (3)	1.20294 (15)	0.48049 (14)	0.0186 (5)
H24	−0.012656	1.203249	0.481615	0.022*
C25	−0.2099 (3)	1.25129 (15)	0.44782 (14)	0.0189 (5)
H25	−0.154262	1.285731	0.426292	0.023*
C26	−0.3758 (3)	1.25043 (15)	0.44591 (14)	0.0189 (5)
H26	−0.429872	1.284470	0.423194	0.023*
C27	−0.4633 (3)	1.20121 (15)	0.47629 (14)	0.0185 (5)
H27	−0.575825	1.200557	0.474834	0.022*
C28	−0.3778 (3)	1.15290 (14)	0.50896 (13)	0.0147 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01909 (8)	0.01702 (9)	0.02029 (9)	0.00047 (6)	−0.00052 (6)	0.00538 (7)
I2	0.02488 (9)	0.02320 (9)	0.01763 (9)	0.00734 (7)	0.00435 (7)	0.00505 (7)
F29	0.0267 (8)	0.0243 (9)	0.0207 (8)	0.0015 (6)	0.0077 (6)	0.0105 (7)
F30	0.0389 (9)	0.0165 (8)	0.0242 (9)	0.0008 (7)	0.0055 (7)	0.0085 (7)
F31	0.0365 (9)	0.0267 (9)	0.0217 (8)	−0.0001 (7)	0.0121 (7)	0.0112 (7)
F32	0.0259 (8)	0.0241 (9)	0.0192 (8)	0.0051 (6)	0.0067 (6)	0.0034 (7)
C29	0.0157 (12)	0.0150 (13)	0.0176 (13)	0.0003 (9)	−0.0012 (9)	0.0052 (11)
C30	0.0148 (12)	0.0233 (14)	0.0179 (13)	0.0010 (10)	0.0011 (10)	0.0080 (11)
C31	0.0165 (12)	0.0192 (14)	0.0134 (12)	0.0051 (10)	0.0015 (9)	0.0035 (10)
C32	0.0210 (13)	0.0174 (14)	0.0185 (13)	0.0012 (10)	−0.0005 (10)	0.0074 (11)
C33	0.0193 (13)	0.0244 (15)	0.0167 (13)	0.0000 (10)	0.0034 (10)	0.0098 (11)
C34	0.0151 (12)	0.0228 (14)	0.0154 (13)	0.0019 (10)	0.0009 (9)	0.0030 (11)
I3	0.03176 (10)	0.02680 (10)	0.01832 (9)	0.00506 (7)	0.00720 (7)	0.00377 (8)

I4	0.02547 (9)	0.01905 (9)	0.02967 (10)	0.00413 (7)	−0.00068 (7)	0.00011 (8)
F33	0.0386 (9)	0.0238 (9)	0.0252 (9)	0.0027 (7)	0.0080 (7)	0.0127 (7)
F34	0.0306 (9)	0.0367 (10)	0.0183 (8)	0.0053 (7)	0.0094 (7)	0.0040 (7)
F35	0.0325 (9)	0.0313 (10)	0.0308 (9)	−0.0031 (7)	0.0084 (7)	0.0182 (8)
F36	0.0261 (8)	0.0155 (8)	0.0351 (10)	0.0008 (6)	0.0060 (7)	0.0067 (7)
C35	0.0159 (12)	0.0174 (14)	0.0218 (14)	0.0018 (10)	−0.0004 (10)	0.0029 (11)
C36	0.0178 (12)	0.0221 (14)	0.0190 (13)	−0.0006 (10)	−0.0005 (10)	0.0090 (11)
C37	0.0169 (12)	0.0206 (14)	0.0149 (13)	0.0025 (10)	0.0004 (9)	0.0035 (11)
C38	0.0142 (12)	0.0180 (14)	0.0243 (14)	0.0006 (10)	−0.0012 (10)	0.0048 (11)
C39	0.0181 (13)	0.0272 (15)	0.0201 (14)	−0.0035 (10)	0.0008 (10)	0.0116 (12)
C40	0.0159 (12)	0.0275 (15)	0.0151 (13)	0.0007 (10)	0.0017 (10)	0.0039 (11)
I5	0.02794 (9)	0.02317 (10)	0.01987 (9)	0.00810 (7)	0.00031 (7)	−0.00193 (7)
I6	0.01777 (8)	0.01347 (8)	0.02020 (9)	−0.00095 (6)	−0.00012 (6)	0.00532 (7)
F37	0.0293 (8)	0.0248 (9)	0.0215 (8)	0.0003 (7)	0.0103 (6)	0.0092 (7)
F38	0.0267 (8)	0.0201 (8)	0.0186 (8)	0.0047 (6)	0.0078 (6)	0.0039 (7)
F39	0.0332 (9)	0.0240 (9)	0.0274 (9)	0.0000 (7)	0.0085 (7)	0.0158 (7)
F40	0.0338 (9)	0.0131 (8)	0.0291 (9)	−0.0013 (6)	−0.0028 (7)	0.0066 (7)
C41	0.0172 (12)	0.0161 (13)	0.0151 (13)	0.0049 (10)	−0.0016 (9)	0.0011 (10)
C42	0.0149 (12)	0.0198 (14)	0.0155 (13)	0.0007 (10)	0.0013 (9)	0.0064 (11)
C43	0.0149 (12)	0.0125 (12)	0.0174 (13)	0.0015 (9)	−0.0011 (9)	0.0049 (10)
C44	0.0162 (12)	0.0176 (13)	0.0161 (13)	0.0027 (10)	0.0006 (9)	0.0041 (11)
C45	0.0182 (12)	0.0182 (14)	0.0195 (13)	−0.0002 (10)	0.0004 (10)	0.0090 (11)
C46	0.0213 (13)	0.0106 (13)	0.0217 (14)	−0.0014 (10)	−0.0053 (10)	0.0050 (11)
S1	0.0117 (3)	0.0187 (3)	0.0194 (3)	0.0011 (2)	0.0010 (2)	0.0057 (3)
N1	0.0100 (10)	0.0206 (12)	0.0150 (11)	0.0013 (8)	0.0013 (8)	0.0037 (9)
N2	0.0094 (10)	0.0198 (12)	0.0169 (11)	0.0021 (8)	0.0008 (8)	0.0057 (9)
C1	0.0141 (12)	0.0179 (13)	0.0123 (12)	0.0001 (9)	0.0015 (9)	−0.0002 (10)
C2	0.0142 (12)	0.0165 (13)	0.0125 (12)	0.0001 (9)	−0.0003 (9)	0.0001 (10)
C3	0.0141 (12)	0.0223 (14)	0.0182 (13)	0.0028 (10)	0.0003 (10)	0.0029 (11)
C4	0.0229 (13)	0.0214 (14)	0.0178 (13)	0.0037 (11)	−0.0007 (10)	0.0052 (11)
C5	0.0235 (13)	0.0191 (14)	0.0148 (13)	−0.0021 (10)	0.0026 (10)	0.0026 (11)
C6	0.0163 (12)	0.0203 (14)	0.0157 (13)	−0.0001 (10)	0.0015 (10)	0.0019 (11)
C7	0.0165 (12)	0.0174 (13)	0.0127 (12)	0.0013 (10)	−0.0010 (9)	0.0029 (10)
S2	0.0118 (3)	0.0130 (3)	0.0192 (3)	0.0003 (2)	0.0004 (2)	0.0054 (3)
N3	0.0096 (10)	0.0158 (11)	0.0180 (11)	0.0016 (8)	0.0003 (8)	0.0061 (9)
N4	0.0112 (10)	0.0133 (11)	0.0153 (11)	0.0011 (8)	0.0004 (8)	0.0036 (9)
C8	0.0126 (11)	0.0128 (12)	0.0127 (12)	0.0017 (9)	0.0000 (9)	0.0004 (10)
C9	0.0154 (12)	0.0147 (13)	0.0138 (12)	0.0003 (9)	0.0011 (9)	0.0030 (10)
C10	0.0148 (12)	0.0200 (14)	0.0208 (14)	−0.0018 (10)	0.0018 (10)	0.0058 (11)
C11	0.0216 (13)	0.0173 (14)	0.0221 (14)	−0.0012 (10)	0.0041 (10)	0.0079 (11)
C12	0.0231 (13)	0.0154 (13)	0.0167 (13)	0.0030 (10)	−0.0006 (10)	0.0045 (11)
C13	0.0146 (12)	0.0164 (13)	0.0147 (12)	0.0044 (9)	0.0019 (9)	0.0003 (10)
C14	0.0143 (11)	0.0126 (12)	0.0132 (12)	−0.0006 (9)	0.0027 (9)	0.0022 (10)
S3	0.0129 (3)	0.0165 (3)	0.0224 (3)	0.0008 (2)	0.0024 (2)	0.0079 (3)
N5	0.0123 (10)	0.0155 (11)	0.0178 (11)	0.0017 (8)	0.0011 (8)	0.0042 (9)
N6	0.0103 (10)	0.0145 (11)	0.0194 (11)	0.0007 (8)	0.0007 (8)	0.0043 (9)
C15	0.0139 (11)	0.0145 (13)	0.0142 (12)	0.0017 (9)	0.0023 (9)	0.0015 (10)
C16	0.0165 (12)	0.0135 (13)	0.0118 (12)	0.0002 (9)	−0.0012 (9)	−0.0005 (10)

C17	0.0189 (13)	0.0204 (14)	0.0163 (13)	0.0065 (10)	−0.0022 (10)	0.0003 (11)
C18	0.0306 (14)	0.0167 (14)	0.0141 (13)	0.0056 (11)	−0.0041 (10)	0.0022 (11)
C19	0.0300 (14)	0.0166 (14)	0.0179 (14)	−0.0005 (11)	0.0020 (11)	0.0063 (11)
C20	0.0206 (13)	0.0167 (13)	0.0165 (13)	−0.0009 (10)	0.0015 (10)	0.0020 (11)
C21	0.0158 (12)	0.0137 (12)	0.0108 (12)	0.0019 (9)	−0.0008 (9)	0.0007 (10)
S4	0.0130 (3)	0.0184 (3)	0.0182 (3)	−0.0002 (2)	0.0001 (2)	0.0078 (3)
N7	0.0114 (10)	0.0195 (12)	0.0159 (11)	−0.0007 (8)	−0.0008 (8)	0.0054 (9)
N8	0.0111 (10)	0.0199 (12)	0.0168 (11)	−0.0001 (8)	0.0016 (8)	0.0070 (9)
C22	0.0146 (12)	0.0152 (13)	0.0119 (12)	0.0007 (9)	−0.0003 (9)	0.0007 (10)
C23	0.0166 (12)	0.0127 (12)	0.0110 (12)	0.0000 (9)	0.0001 (9)	−0.0011 (10)
C24	0.0182 (12)	0.0192 (14)	0.0164 (13)	−0.0050 (10)	0.0018 (10)	0.0028 (11)
C25	0.0254 (13)	0.0141 (13)	0.0169 (13)	−0.0022 (10)	0.0030 (10)	0.0044 (11)
C26	0.0242 (13)	0.0166 (13)	0.0153 (13)	0.0017 (10)	0.0009 (10)	0.0037 (11)
C27	0.0164 (12)	0.0191 (14)	0.0187 (13)	0.0018 (10)	0.0005 (10)	0.0035 (11)
C28	0.0162 (12)	0.0134 (12)	0.0143 (12)	−0.0012 (9)	0.0016 (9)	0.0037 (10)

Geometric parameters (Å, º)

I1—C29	2.090 (3)	C6—C7	1.390 (3)
I2—C31	2.088 (2)	S2—C8	1.696 (2)
F29—C30	1.348 (3)	N3—HN3	0.846 (17)
F30—C32	1.342 (3)	N3—C8	1.354 (3)
F31—C33	1.344 (3)	N3—C9	1.394 (3)
F32—C34	1.343 (3)	N4—HN4	0.849 (16)
C29—C30	1.392 (3)	N4—C8	1.356 (3)
C29—C34	1.387 (3)	N4—C14	1.390 (3)
C30—C31	1.382 (4)	C9—C10	1.388 (3)
C31—C32	1.387 (3)	C9—C14	1.398 (3)
C32—C33	1.382 (4)	C10—H10	0.9500
C33—C34	1.378 (4)	C10—C11	1.390 (3)
I3—C37	2.083 (2)	C11—H11	0.9500
I4—C35	2.082 (3)	C11—C12	1.394 (3)
F33—C36	1.343 (3)	C12—H12	0.9500
F34—C40	1.344 (3)	C12—C13	1.391 (4)
F35—C39	1.342 (3)	C13—H13	0.9500
F36—C38	1.342 (3)	C13—C14	1.388 (3)
C35—C36	1.390 (4)	S3—C15	1.699 (2)
C35—C40	1.389 (4)	N5—HN5	0.850 (17)
C36—C37	1.386 (4)	N5—C15	1.360 (3)
C37—C38	1.385 (4)	N5—C16	1.388 (3)
C38—C39	1.383 (4)	N6—HN6	0.851 (17)
C39—C40	1.373 (4)	N6—C15	1.348 (3)
I5—C41	2.092 (2)	N6—C21	1.390 (3)
I6—C43	2.088 (2)	C16—C17	1.394 (3)
F37—C42	1.347 (3)	C16—C21	1.398 (3)
F38—C44	1.345 (3)	C17—H17	0.9500
F39—C45	1.344 (3)	C17—C18	1.386 (4)
F40—C46	1.343 (3)	C18—H18	0.9500

C41—C42	1.379 (4)	C18—C19	1.396 (4)
C41—C46	1.382 (4)	C19—H19	0.9500
C42—C43	1.390 (3)	C19—C20	1.387 (3)
C43—C44	1.382 (3)	C20—H20	0.9500
C44—C45	1.377 (4)	C20—C21	1.386 (3)
C45—C46	1.378 (4)	S4—C22	1.693 (2)
S1—C1	1.693 (3)	N7—HN7	0.844 (17)
N1—HN1	0.847 (17)	N7—C22	1.358 (3)
N1—C1	1.358 (3)	N7—C23	1.391 (3)
N1—C2	1.390 (3)	N8—HN8	0.852 (17)
N2—HN2	0.854 (16)	N8—C22	1.353 (3)
N2—C1	1.358 (3)	N8—C28	1.389 (3)
N2—C7	1.390 (3)	C23—C24	1.386 (3)
C2—C3	1.385 (3)	C23—C28	1.398 (3)
C2—C7	1.404 (3)	C24—H24	0.9500
C3—H3	0.9500	C24—C25	1.388 (3)
C3—C4	1.384 (4)	C25—H25	0.9500
C4—H4	0.9500	C25—C26	1.401 (3)
C4—C5	1.402 (3)	C26—H26	0.9500
C5—H5	0.9500	C26—C27	1.388 (4)
C5—C6	1.390 (3)	C27—H27	0.9500
C6—H6	0.9500	C27—C28	1.390 (3)

C30—C29—I1	121.55 (18)	C8—N3—HN3	123 (2)
C34—C29—I1	120.98 (19)	C8—N3—C9	110.03 (19)
C34—C29—C30	117.4 (2)	C9—N3—HN3	126 (2)
F29—C30—C29	118.4 (2)	C8—N4—HN4	122.6 (18)
F29—C30—C31	118.6 (2)	C8—N4—C14	109.91 (19)
C31—C30—C29	123.0 (2)	C14—N4—HN4	126.3 (18)
C30—C31—I2	121.81 (18)	N3—C8—S2	126.82 (17)
C30—C31—C32	117.5 (2)	N3—C8—N4	107.3 (2)
C32—C31—I2	120.72 (19)	N4—C8—S2	125.90 (18)
F30—C32—C31	120.7 (2)	N3—C9—C14	106.2 (2)
F30—C32—C33	118.0 (2)	C10—C9—N3	132.1 (2)
C33—C32—C31	121.3 (2)	C10—C9—C14	121.7 (2)
F31—C33—C32	120.0 (2)	C9—C10—H10	121.9
F31—C33—C34	120.4 (2)	C9—C10—C11	116.3 (2)
C34—C33—C32	119.6 (2)	C11—C10—H10	121.9
F32—C34—C29	120.3 (2)	C10—C11—H11	119.0
F32—C34—C33	118.5 (2)	C10—C11—C12	122.1 (2)
C33—C34—C29	121.2 (2)	C12—C11—H11	119.0
C36—C35—I4	122.13 (19)	C11—C12—H12	119.2
C40—C35—I4	120.40 (19)	C13—C12—C11	121.6 (2)
C40—C35—C36	117.4 (2)	C13—C12—H12	119.2
F33—C36—C35	118.6 (2)	C12—C13—H13	121.8
F33—C36—C37	118.7 (2)	C14—C13—C12	116.4 (2)
C37—C36—C35	122.7 (2)	C14—C13—H13	121.8
C36—C37—I3	121.94 (19)	N4—C14—C9	106.5 (2)

C38—C37—I3	120.42 (19)	C13—C14—N4	131.5 (2)
C38—C37—C36	117.6 (2)	C13—C14—C9	121.9 (2)
F36—C38—C37	120.2 (2)	C15—N5—HN5	122 (2)
F36—C38—C39	118.4 (2)	C15—N5—C16	109.8 (2)
C39—C38—C37	121.4 (2)	C16—N5—HN5	128 (2)
F35—C39—C38	120.0 (2)	C15—N6—HN6	125.4 (19)
F35—C39—C40	120.6 (2)	C15—N6—C21	110.28 (19)
C40—C39—C38	119.4 (2)	C21—N6—HN6	124.0 (19)
F34—C40—C35	120.2 (2)	N5—C15—S3	126.48 (18)
F34—C40—C39	118.3 (2)	N6—C15—S3	126.32 (18)
C39—C40—C35	121.5 (2)	N6—C15—N5	107.2 (2)
C42—C41—I5	122.49 (18)	N5—C16—C17	132.2 (2)
C42—C41—C46	117.7 (2)	N5—C16—C21	106.5 (2)
C46—C41—I5	119.79 (19)	C17—C16—C21	121.2 (2)
F37—C42—C41	119.0 (2)	C16—C17—H17	121.8
F37—C42—C43	118.4 (2)	C18—C17—C16	116.4 (2)
C41—C42—C43	122.6 (2)	C18—C17—H17	121.8
C42—C43—I6	122.78 (18)	C17—C18—H18	119.1
C44—C43—I6	119.64 (18)	C17—C18—C19	121.9 (2)
C44—C43—C42	117.6 (2)	C19—C18—H18	119.1
F38—C44—C43	120.5 (2)	C18—C19—H19	119.0
F38—C44—C45	118.2 (2)	C20—C19—C18	122.0 (2)
C45—C44—C43	121.4 (2)	C20—C19—H19	119.0
F39—C45—C44	120.0 (2)	C19—C20—H20	122.0
F39—C45—C46	120.8 (2)	C21—C20—C19	116.1 (2)
C44—C45—C46	119.3 (2)	C21—C20—H20	122.0
F40—C46—C41	120.7 (2)	N6—C21—C16	106.2 (2)
F40—C46—C45	117.8 (2)	C20—C21—N6	131.4 (2)
C45—C46—C41	121.5 (2)	C20—C21—C16	122.4 (2)
C1—N1—HN1	123 (2)	C22—N7—HN7	124 (2)
C1—N1—C2	110.7 (2)	C22—N7—C23	110.29 (19)
C2—N1—HN1	126 (2)	C23—N7—HN7	125 (2)
C1—N2—HN2	124.7 (18)	C22—N8—HN8	122 (2)
C1—N2—C7	110.48 (19)	C22—N8—C28	110.6 (2)
C7—N2—HN2	124.7 (18)	C28—N8—HN8	127 (2)
N1—C1—S1	127.03 (19)	N7—C22—S4	126.72 (18)
N1—C1—N2	106.5 (2)	N8—C22—S4	126.58 (18)
N2—C1—S1	126.41 (18)	N8—C22—N7	106.7 (2)
N1—C2—C7	106.0 (2)	N7—C23—C28	106.2 (2)
C3—C2—N1	132.4 (2)	C24—C23—N7	132.1 (2)
C3—C2—C7	121.6 (2)	C24—C23—C28	121.6 (2)
C2—C3—H3	121.5	C23—C24—H24	121.5
C4—C3—C2	116.9 (2)	C23—C24—C25	116.9 (2)
C4—C3—H3	121.5	C25—C24—H24	121.5
C3—C4—H4	119.2	C24—C25—H25	119.3
C3—C4—C5	121.6 (2)	C24—C25—C26	121.4 (2)
C5—C4—H4	119.2	C26—C25—H25	119.3
C4—C5—H5	119.1	C25—C26—H26	119.1

C6—C5—C4	121.8 (2)	C27—C26—C25	121.8 (2)
C6—C5—H5	119.1	C27—C26—H26	119.1
C5—C6—H6	121.8	C26—C27—H27	121.7
C7—C6—C5	116.5 (2)	C26—C27—C28	116.5 (2)
C7—C6—H6	121.8	C28—C27—H27	121.7
N2—C7—C2	106.3 (2)	N8—C28—C23	106.2 (2)
N2—C7—C6	132.0 (2)	N8—C28—C27	132.1 (2)
C6—C7—C2	121.6 (2)	C27—C28—C23	121.7 (2)
I1—C29—C30—F29	1.8 (3)	N1—C2—C7—C6	−177.7 (2)
I1—C29—C30—C31	−178.02 (18)	C1—N1—C2—C3	−177.6 (3)
I1—C29—C34—F32	−0.7 (3)	C1—N1—C2—C7	−0.7 (3)
I1—C29—C34—C33	178.45 (19)	C1—N2—C7—C2	0.1 (3)
I2—C31—C32—F30	−1.4 (3)	C1—N2—C7—C6	177.9 (3)
I2—C31—C32—C33	179.38 (19)	C2—N1—C1—S1	179.67 (19)
F29—C30—C31—I2	0.8 (3)	C2—N1—C1—N2	0.8 (3)
F29—C30—C31—C32	179.9 (2)	C2—C3—C4—C5	0.2 (4)
F30—C32—C33—F31	0.7 (4)	C3—C2—C7—N2	177.6 (2)
F30—C32—C33—C34	−179.2 (2)	C3—C2—C7—C6	−0.5 (4)
F31—C33—C34—F32	−1.3 (4)	C3—C4—C5—C6	−0.4 (4)
F31—C33—C34—C29	179.6 (2)	C4—C5—C6—C7	0.2 (4)
C29—C30—C31—I2	−179.37 (18)	C5—C6—C7—N2	−177.3 (3)
C29—C30—C31—C32	−0.3 (4)	C5—C6—C7—C2	0.2 (4)
C30—C29—C34—F32	−178.6 (2)	C7—N2—C1—S1	−179.44 (19)
C30—C29—C34—C33	0.5 (4)	C7—N2—C1—N1	−0.6 (3)
C30—C31—C32—F30	179.5 (2)	C7—C2—C3—C4	0.2 (4)
C30—C31—C32—C33	0.3 (4)	N3—C9—C10—C11	177.7 (3)
C31—C32—C33—F31	180.0 (2)	N3—C9—C14—N4	0.1 (3)
C31—C32—C33—C34	0.1 (4)	N3—C9—C14—C13	−176.7 (2)
C32—C33—C34—F32	178.6 (2)	C8—N3—C9—C10	179.5 (3)
C32—C33—C34—C29	−0.5 (4)	C8—N3—C9—C14	−1.5 (3)
C34—C29—C30—F29	179.7 (2)	C8—N4—C14—C9	1.3 (3)
C34—C29—C30—C31	−0.1 (4)	C8—N4—C14—C13	177.6 (3)
I3—C37—C38—F36	3.5 (3)	C9—N3—C8—S2	−176.81 (19)
I3—C37—C38—C39	−175.80 (19)	C9—N3—C8—N4	2.3 (3)
I4—C35—C36—F33	−3.1 (3)	C9—C10—C11—C12	−0.7 (4)
I4—C35—C36—C37	177.10 (19)	C10—C9—C14—N4	179.3 (2)
I4—C35—C40—F34	3.5 (3)	C10—C9—C14—C13	2.5 (4)
I4—C35—C40—C39	−175.96 (19)	C10—C11—C12—C13	1.6 (4)
F33—C36—C37—I3	−3.5 (3)	C11—C12—C13—C14	−0.4 (4)
F33—C36—C37—C38	179.1 (2)	C12—C13—C14—N4	−177.5 (2)
F35—C39—C40—F34	−0.8 (4)	C12—C13—C14—C9	−1.6 (4)
F35—C39—C40—C35	178.7 (2)	C14—N4—C8—S2	176.89 (18)
F36—C38—C39—F35	0.3 (4)	C14—N4—C8—N3	−2.2 (3)
F36—C38—C39—C40	−179.9 (2)	C14—C9—C10—C11	−1.3 (4)
C35—C36—C37—I3	176.28 (19)	N5—C16—C17—C18	179.3 (3)
C35—C36—C37—C38	−1.2 (4)	N5—C16—C21—N6	−0.4 (3)
C36—C35—C40—F34	−178.9 (2)	N5—C16—C21—C20	−179.2 (2)

C36—C35—C40—C39	1.6 (4)	C15—N5—C16—C17	−179.3 (3)
C36—C37—C38—F36	−179.0 (2)	C15—N5—C16—C21	−0.6 (3)
C36—C37—C38—C39	1.7 (4)	C15—N6—C21—C16	1.2 (3)
C37—C38—C39—F35	179.6 (2)	C15—N6—C21—C20	179.8 (3)
C37—C38—C39—C40	−0.6 (4)	C16—N5—C15—S3	−177.01 (19)
C38—C39—C40—F34	179.4 (2)	C16—N5—C15—N6	1.3 (3)
C38—C39—C40—C35	−1.1 (4)	C16—C17—C18—C19	−0.3 (4)
C40—C35—C36—F33	179.3 (2)	C17—C16—C21—N6	178.5 (2)
C40—C35—C36—C37	−0.4 (4)	C17—C16—C21—C20	−0.3 (4)
I5—C41—C42—F37	−3.0 (3)	C17—C18—C19—C20	−0.7 (4)
I5—C41—C42—C43	177.25 (18)	C18—C19—C20—C21	1.2 (4)
I5—C41—C46—F40	0.8 (3)	C19—C20—C21—N6	−179.1 (2)
I5—C41—C46—C45	−178.55 (18)	C19—C20—C21—C16	−0.7 (4)
I6—C43—C44—F38	−2.9 (3)	C21—N6—C15—S3	176.77 (19)
I6—C43—C44—C45	177.54 (18)	C21—N6—C15—N5	−1.6 (3)
F37—C42—C43—I6	2.7 (3)	C21—C16—C17—C18	0.8 (4)
F37—C42—C43—C44	−178.6 (2)	N7—C23—C24—C25	179.5 (2)
F38—C44—C45—F39	1.2 (3)	N7—C23—C28—N8	−0.2 (3)
F38—C44—C45—C46	−179.6 (2)	N7—C23—C28—C27	−179.8 (2)
F39—C45—C46—F40	1.2 (3)	C22—N7—C23—C24	−179.2 (3)
F39—C45—C46—C41	−179.4 (2)	C22—N7—C23—C28	−0.3 (3)
C41—C42—C43—I6	−177.57 (18)	C22—N8—C28—C23	0.7 (3)
C41—C42—C43—C44	1.1 (4)	C22—N8—C28—C27	−179.8 (3)
C42—C41—C46—F40	178.0 (2)	C23—N7—C22—S4	179.87 (19)
C42—C41—C46—C45	−1.3 (4)	C23—N7—C22—N8	0.8 (3)
C42—C43—C44—F38	178.4 (2)	C23—C24—C25—C26	−0.3 (4)
C42—C43—C44—C45	−1.2 (4)	C24—C23—C28—N8	178.7 (2)
C43—C44—C45—F39	−179.2 (2)	C24—C23—C28—C27	−0.8 (4)
C43—C44—C45—C46	0.0 (4)	C24—C25—C26—C27	−0.2 (4)
C44—C45—C46—F40	−178.1 (2)	C25—C26—C27—C28	0.2 (4)
C44—C45—C46—C41	1.3 (4)	C26—C27—C28—N8	−179.1 (3)
C46—C41—C42—F37	179.8 (2)	C26—C27—C28—C23	0.3 (4)
C46—C41—C42—C43	0.1 (4)	C28—N8—C22—S4	179.97 (19)
N1—C2—C3—C4	176.7 (3)	C28—N8—C22—N7	−1.0 (3)
N1—C2—C7—N2	0.4 (3)	C28—C23—C24—C25	0.8 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···S2^{i}	0.85 (2)	2.52 (2)	3.357 (2)	172 (3)
N2—H*N*2···S2	0.85 (2)	2.46 (2)	3.297 (2)	166 (2)
N3—H*N*3···S1	0.85 (2)	2.51 (2)	3.348 (2)	173 (3)
N4—H*N*4···S1^{ii}	0.85 (2)	2.50 (2)	3.326 (2)	166 (2)
N5—H*N*5···S4^{i}	0.85 (2)	2.49 (2)	3.326 (2)	169 (3)
N6—H*N*6···S4	0.85 (2)	2.43 (2)	3.270 (2)	169 (3)
C17—H17···F36^{iii}	0.95	2.61	3.385 (3)	139
C20—H20···F36^{iv}	0.95	2.51	3.235 (3)	133

N7—H*N*7···S3	0.84 (2)	2.47 (2)	3.300 (2)	170 (3)
N8—H*N*8···S3^{ii}	0.85 (2)	2.48 (2)	3.302 (2)	163 (3)

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

1*H*-1,3-Benzodiazole-2-thiol–1,2,4,5-tetrafluoro-3,6-diiodobenzene (1/1) (MBZIM_14F4DIB)

Crystal data

$C_6F_4I_2·C_7H_6N_2S$
M_r = 552.06
Monoclinic, $P2_1/c$
a = 5.5641 (2) Å
b = 33.1320 (11) Å
c = 8.4710 (3) Å
β = 92.754 (1)°
V = 1559.82 (9) Å^3
Z = 4
F(000) = 1024
D_x = 2.351 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 9812 reflections
θ = 2.5–30.2°
μ = 4.20 mm^{-1}
T = 100 K
Plate, colourless
0.22 × 0.18 × 0.06 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec I*μ*S
φ and *ω* scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.501, T_{max} = 0.746
45583 measured reflections
4579 independent reflections
4211 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 30.2°, θ_{min} = 2.5°
h = −7→7
k = −46→46
l = −11→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.044
S = 1.12
4579 reflections
207 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0059P)^2 + 1.8833P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.67 e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.61301 (2)	0.38195 (2)	0.76376 (2)	0.01796 (4)
I2	0.89550 (3)	0.17772 (2)	0.69482 (2)	0.02372 (4)
F1	1.0451 (2)	0.33570 (4)	0.60867 (16)	0.0251 (3)
F2	1.1463 (3)	0.25762 (4)	0.57675 (17)	0.0283 (3)
F3	0.4636 (3)	0.22323 (4)	0.85802 (18)	0.0292 (3)
F4	0.3576 (2)	0.30171 (4)	0.88704 (18)	0.0285 (3)

C8	0.6955 (4)	0.32080 (6)	0.7457 (2)	0.0160 (4)
C9	0.8965 (4)	0.30829 (6)	0.6680 (2)	0.0176 (4)
C10	0.9499 (4)	0.26788 (7)	0.6526 (2)	0.0182 (4)
C11	0.8062 (4)	0.23834 (6)	0.7151 (2)	0.0174 (4)
C12	0.6066 (4)	0.25062 (7)	0.7940 (3)	0.0188 (4)
C13	0.5531 (4)	0.29113 (7)	0.8091 (3)	0.0193 (4)
S1	0.58078 (9)	0.48006 (2)	0.75000 (6)	0.01583 (10)
N1	0.2303 (3)	0.52614 (5)	0.8744 (2)	0.0153 (3)
HN1	0.276 (5)	0.5218 (8)	0.969 (3)	0.023 (7)*
N2	0.2252 (3)	0.52735 (5)	0.6175 (2)	0.0149 (3)
HN2	0.276 (5)	0.5229 (8)	0.525 (3)	0.023 (7)*
C1	0.3405 (4)	0.51181 (6)	0.7471 (2)	0.0143 (4)
C2	0.0446 (4)	0.55224 (6)	0.8266 (2)	0.0147 (4)
C3	−0.1194 (4)	0.57380 (6)	0.9113 (2)	0.0180 (4)
H00G	−0.116250	0.573127	1.023460	0.022*
C4	−0.2889 (4)	0.59651 (7)	0.8238 (3)	0.0196 (4)
H00M	−0.404740	0.611727	0.877214	0.024*
C5	−0.2920 (4)	0.59733 (7)	0.6581 (3)	0.0203 (4)
H00J	−0.409996	0.613183	0.602105	0.024*
C6	−0.1275 (4)	0.57565 (6)	0.5737 (2)	0.0186 (4)
H00L	−0.130222	0.576283	0.461502	0.022*
C7	0.0408 (4)	0.55303 (6)	0.6613 (2)	0.0147 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.02099 (7)	0.01539 (7)	0.01731 (7)	0.00072 (5)	−0.00093 (5)	−0.00014 (5)
I2	0.03021 (8)	0.01541 (7)	0.02536 (8)	0.00224 (6)	−0.00059 (6)	−0.00099 (5)
F1	0.0259 (7)	0.0215 (6)	0.0286 (7)	−0.0048 (6)	0.0099 (6)	0.0039 (5)
F2	0.0264 (7)	0.0260 (7)	0.0339 (8)	0.0022 (6)	0.0152 (6)	−0.0012 (6)
F3	0.0255 (7)	0.0191 (7)	0.0440 (9)	−0.0047 (6)	0.0132 (6)	0.0058 (6)
F4	0.0222 (7)	0.0248 (7)	0.0400 (8)	0.0019 (6)	0.0160 (6)	0.0021 (6)
C8	0.0175 (9)	0.0145 (9)	0.0159 (9)	0.0007 (8)	−0.0011 (7)	−0.0006 (7)
C9	0.0195 (10)	0.0183 (10)	0.0151 (9)	−0.0039 (8)	0.0025 (8)	0.0026 (7)
C10	0.0171 (10)	0.0210 (10)	0.0169 (9)	0.0011 (8)	0.0036 (8)	−0.0004 (8)
C11	0.0199 (10)	0.0146 (9)	0.0174 (10)	−0.0004 (8)	−0.0018 (8)	−0.0009 (7)
C12	0.0187 (10)	0.0178 (10)	0.0200 (10)	−0.0040 (8)	0.0030 (8)	0.0013 (8)
C13	0.0172 (10)	0.0202 (10)	0.0207 (10)	0.0021 (8)	0.0041 (8)	−0.0001 (8)
S1	0.0208 (2)	0.0150 (2)	0.0116 (2)	0.00308 (19)	0.00018 (18)	−0.00025 (16)
N1	0.0177 (8)	0.0184 (8)	0.0096 (8)	0.0020 (7)	−0.0017 (6)	−0.0003 (6)
N2	0.0175 (8)	0.0172 (8)	0.0101 (8)	0.0005 (7)	0.0010 (6)	−0.0007 (6)
C1	0.0180 (9)	0.0129 (9)	0.0119 (8)	−0.0026 (8)	−0.0003 (7)	−0.0004 (7)
C2	0.0150 (9)	0.0152 (9)	0.0139 (9)	−0.0016 (8)	−0.0011 (7)	0.0003 (7)
C3	0.0198 (10)	0.0191 (10)	0.0151 (9)	−0.0017 (8)	0.0010 (8)	−0.0029 (7)
C4	0.0182 (10)	0.0201 (10)	0.0206 (10)	0.0009 (8)	0.0021 (8)	−0.0022 (8)
C5	0.0191 (10)	0.0186 (10)	0.0229 (11)	0.0009 (8)	−0.0017 (8)	0.0021 (8)
C6	0.0203 (10)	0.0212 (10)	0.0139 (9)	0.0000 (8)	−0.0021 (8)	0.0021 (7)
C7	0.0158 (9)	0.0158 (9)	0.0125 (9)	−0.0017 (8)	−0.0006 (7)	−0.0007 (7)

Geometric parameters (Å, º)

I1—C8	2.084 (2)	N1—C2	1.393 (3)
I2—C11	2.078 (2)	N2—HN2	0.86 (3)
F1—C9	1.342 (2)	N2—C1	1.347 (3)
F2—C10	1.338 (2)	N2—C7	1.397 (3)
F3—C12	1.338 (2)	C2—C3	1.385 (3)
F4—C13	1.346 (2)	C2—C7	1.400 (3)
C8—C9	1.388 (3)	C3—H00G	0.9500
C8—C13	1.387 (3)	C3—C4	1.392 (3)
C9—C10	1.379 (3)	C4—H00M	0.9500
C10—C11	1.386 (3)	C4—C5	1.402 (3)
C11—C12	1.384 (3)	C5—H00J	0.9500
C12—C13	1.382 (3)	C5—C6	1.388 (3)
S1—C1	1.700 (2)	C6—H00L	0.9500
N1—HN1	0.84 (3)	C6—C7	1.387 (3)
N1—C1	1.352 (2)		

C9—C8—I1	120.68 (15)	C7—N2—HN2	128.7 (18)
C13—C8—I1	121.91 (15)	N1—C1—S1	126.31 (16)
C13—C8—C9	117.41 (19)	N2—C1—S1	126.27 (15)
F1—C9—C8	120.03 (19)	N2—C1—N1	107.42 (18)
F1—C9—C10	118.85 (18)	N1—C2—C7	106.11 (17)
C10—C9—C8	121.11 (19)	C3—C2—N1	131.90 (19)
F2—C10—C9	118.48 (19)	C3—C2—C7	121.97 (19)
F2—C10—C11	120.25 (19)	C2—C3—H00G	121.6
C9—C10—C11	121.27 (19)	C2—C3—C4	116.70 (19)
C10—C11—I2	120.42 (15)	C4—C3—H00G	121.6
C12—C11—I2	121.65 (16)	C3—C4—H00M	119.4
C12—C11—C10	117.92 (19)	C3—C4—C5	121.2 (2)
F3—C12—C11	120.16 (19)	C5—C4—H00M	119.4
F3—C12—C13	119.09 (19)	C4—C5—H00J	119.0
C13—C12—C11	120.75 (19)	C6—C5—C4	121.9 (2)
F4—C13—C8	119.71 (19)	C6—C5—H00J	119.0
F4—C13—C12	118.75 (19)	C5—C6—H00L	121.7
C12—C13—C8	121.54 (19)	C7—C6—C5	116.65 (19)
C1—N1—HN1	125.0 (18)	C7—C6—H00L	121.7
C1—N1—C2	110.19 (17)	N2—C7—C2	106.19 (17)
C2—N1—HN1	124.6 (18)	C6—C7—N2	132.27 (18)
C1—N2—HN2	121.0 (19)	C6—C7—C2	121.53 (19)
C1—N2—C7	110.07 (17)		

I1—C8—C9—F1	2.5 (3)	C13—C8—C9—F1	−177.88 (19)
I1—C8—C9—C10	−178.66 (16)	C13—C8—C9—C10	1.0 (3)
I1—C8—C13—F4	−1.1 (3)	N1—C2—C3—C4	−178.1 (2)
I1—C8—C13—C12	178.80 (17)	N1—C2—C7—N2	−0.1 (2)
I2—C11—C12—F3	−0.8 (3)	N1—C2—C7—C6	178.62 (19)
I2—C11—C12—C13	178.65 (17)	C1—N1—C2—C3	179.2 (2)

F1—C9—C10—F2	−1.0 (3)	C1—N1—C2—C7	1.0 (2)
F1—C9—C10—C11	178.30 (19)	C1—N2—C7—C2	−0.9 (2)
F2—C10—C11—I2	0.8 (3)	C1—N2—C7—C6	−179.4 (2)
F2—C10—C11—C12	179.3 (2)	C2—N1—C1—S1	178.30 (15)
F3—C12—C13—F4	−0.4 (3)	C2—N1—C1—N2	−1.6 (2)
F3—C12—C13—C8	179.7 (2)	C2—C3—C4—C5	0.0 (3)
C8—C9—C10—F2	−179.86 (19)	C3—C2—C7—N2	−178.50 (19)
C8—C9—C10—C11	−0.6 (3)	C3—C2—C7—C6	0.2 (3)
C9—C8—C13—F4	179.28 (19)	C3—C4—C5—C6	0.1 (3)
C9—C8—C13—C12	−0.8 (3)	C4—C5—C6—C7	0.0 (3)
C9—C10—C11—I2	−178.52 (17)	C5—C6—C7—N2	178.2 (2)
C9—C10—C11—C12	0.0 (3)	C5—C6—C7—C2	−0.1 (3)
C10—C11—C12—F3	−179.3 (2)	C7—N2—C1—S1	−178.36 (15)
C10—C11—C12—C13	0.2 (3)	C7—N2—C1—N1	1.5 (2)
C11—C12—C13—F4	−179.8 (2)	C7—C2—C3—C4	−0.1 (3)
C11—C12—C13—C8	0.3 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···S1^{i}	0.84 (3)	2.47 (3)	3.3089 (18)	172 (2)
N2—H*N*2···S1^{ii}	0.86 (3)	2.50 (3)	3.3527 (17)	172 (2)

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

1*H*-1,3-Benzodiazole-2-thiol–1,1,2,2-tetraiodoethene (1/1) (MBZIM_TIE)

Crystal data

$C_2I_4{\cdot}C_7H_6N_2S$
M_r = 681.82
Orthorhombic, *Pnma*
a = 11.7547 (10) Å
b = 8.3525 (7) Å
c = 15.1077 (13) Å
V = 1483.3 (2) Å^3
Z = 4
F(000) = 1208
D_x = 3.053 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 32859 reflections
θ = 2.2–28.5°
μ = 8.52 mm^{-1}
T = 100 K
Plank, colourless
0.30 × 0.14 × 0.11 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec I*μ*S
φ and *ω* scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.256, T_{max} = 0.746
32859 measured reflections
1993 independent reflections
1885 reflections with $I > 2\sigma(I)$
R_{int} = 0.055
θ_{max} = 28.5°, θ_{min} = 2.2°
h = −15→15
k = −11→11
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.062
S = 1.25
1993 reflections
89 parameters
0 restraints

Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0213P)^2 + 6.7951P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.25$ e Å^{-3}
$\Delta\rho_{min} = -1.48$ e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.71885 (3)	0.250000	0.41396 (2)	0.01158 (9)
I2	0.48169 (3)	0.250000	0.27066 (2)	0.01399 (9)
I3	0.29263 (3)	0.250000	0.46197 (2)	0.01401 (9)
I4	0.52953 (3)	0.250000	0.60280 (2)	0.02001 (10)
C5	0.5414 (5)	0.250000	0.4030 (4)	0.0165 (11)
C6	0.4724 (5)	0.250000	0.4721 (4)	0.0174 (11)
S1	1.01449 (11)	0.250000	0.45747 (8)	0.0100 (2)
N1	0.9064 (3)	0.3808 (4)	0.5997 (2)	0.0103 (6)
HN1	0.925 (4)	0.478 (6)	0.586 (3)	0.016 (12)*
C1	0.9436 (4)	0.250000	0.5556 (3)	0.0113 (10)
C2	0.8394 (3)	0.3332 (4)	0.6716 (2)	0.0101 (7)
C3	0.7765 (3)	0.4217 (5)	0.7322 (2)	0.0124 (7)
H3	0.776830	0.535466	0.732234	0.015*
C4	0.7128 (3)	0.3335 (5)	0.7928 (2)	0.0134 (7)
H4	0.668132	0.388696	0.835332	0.016*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.00779 (16)	0.01634 (17)	0.01059 (16)	0.000	−0.00164 (11)	0.000
I2	0.01027 (17)	0.02331 (19)	0.00839 (16)	0.000	−0.00137 (11)	0.000
I3	0.00843 (16)	0.01822 (18)	0.01538 (17)	0.000	0.00119 (12)	0.000
I4	0.01263 (18)	0.0392 (2)	0.00821 (17)	0.000	−0.00150 (12)	0.000
C5	0.012 (3)	0.023 (3)	0.014 (3)	0.000	−0.002 (2)	0.000
C6	0.019 (3)	0.025 (3)	0.008 (2)	0.000	−0.004 (2)	0.000
S1	0.0102 (5)	0.0095 (5)	0.0102 (5)	0.000	0.0029 (4)	0.000
N1	0.0103 (14)	0.0088 (14)	0.0117 (14)	−0.0008 (11)	0.0015 (11)	−0.0004 (11)
C1	0.008 (2)	0.014 (2)	0.012 (2)	0.000	−0.0048 (18)	0.000
C2	0.0090 (15)	0.0123 (18)	0.0090 (15)	0.0000 (13)	−0.0024 (12)	−0.0001 (13)
C3	0.0132 (17)	0.0116 (16)	0.0125 (16)	0.0013 (13)	0.0002 (13)	−0.0011 (13)
C4	0.0109 (16)	0.0172 (19)	0.0119 (16)	0.0023 (14)	0.0030 (13)	−0.0017 (14)

Geometric parameters (Å, º)

I1—C5	2.093 (6)	N1—C2	1.400 (4)
I2—C5	2.119 (6)	C2—C2^{i}	1.390 (7)
I3—C6	2.118 (6)	C2—C3	1.389 (5)
I4—C6	2.086 (5)	C3—H3	0.9500
C5—C6	1.321 (8)	C3—C4	1.393 (5)
S1—C1	1.701 (6)	C4—C4^{i}	1.395 (8)
N1—HN1	0.87 (5)	C4—H4	0.9500
N1—C1	1.352 (4)		
I1—C5—I2	113.9 (3)	N1^{i}—C1—N1	107.8 (5)
C6—C5—I1	123.3 (4)	C2^{i}—C2—N1	106.5 (2)
C6—C5—I2	122.8 (4)	C3—C2—N1	131.3 (3)
I4—C6—I3	112.9 (3)	C3—C2—C2^{i}	122.2 (2)
C5—C6—I3	123.7 (4)	C2—C3—H3	122.1
C5—C6—I4	123.3 (5)	C2—C3—C4	115.9 (3)
C1—N1—HN1	124 (3)	C4—C3—H3	122.1
C1—N1—C2	109.6 (3)	C3—C4—C4^{i}	121.9 (2)
C2—N1—HN1	127 (3)	C3—C4—H4	119.0
N1—C1—S1	126.0 (2)	C4^{i}—C4—H4	119.0
N1^{i}—C1—S1	126.0 (2)		
I1—C5—C6—I3	180.000 (1)	C1—N1—C2—C3	−174.9 (4)
I1—C5—C6—I4	0.000 (1)	C2—N1—C1—S1	172.5 (3)
I2—C5—C6—I3	0.000 (1)	C2—N1—C1—N1^{i}	−2.6 (5)
I2—C5—C6—I4	180.000 (1)	C2^{i}—C2—C3—C4	−0.3 (4)
N1—C2—C3—C4	175.8 (4)	C2—C3—C4—C4^{i}	0.3 (4)
C1—N1—C2—C2^{i}	1.6 (3)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···S1^{ii}	0.87 (5)	2.47 (5)	3.335 (3)	178 (5)
C3—H3···I1^{iii}	0.95	3.28	3.881 (4)	123

Symmetry codes: (ii) −*x*+2, −*y*+1, −*z*+1; (iii) −*x*+3/2, −*y*+1, *z*+1/2.

5-Methyl-1*H*-1,3-benzodiazole-2-thiol–1,2,3,4-tetrafluoro-5,6-diiodobenzene (1/1) (MMBZIM_12F4DIB)

Crystal data

$C_6F_4I_2·C_8H_8N_2S$
M_r = 566.08
Triclinic, $P\overline{1}$
a = 4.5504 (5) Å
b = 13.2872 (14) Å
c = 13.8064 (14) Å
α = 94.766 (4)°
β = 98.124 (4)°
γ = 99.588 (4)°
V = 809.97 (15) Å^3
Z = 2
F(000) = 528
D_x = 2.321 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 9940 reflections
θ = 2.3–27.5°

μ = 4.05 mm^{-1}
T = 100 K

Needle, colourless
0.19 × 0.07 × 0.04 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec IμS
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.636, T_{max} = 0.746
21426 measured reflections

3704 independent reflections
3174 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 27.5°, θ_{min} = 2.3°
h = −5→5
k = −17→17
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.055
S = 1.24
3704 reflections
217 parameters
1 restraint
Primary atom site location: dual

Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + 2.2494P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.33 e Å^{-3}
$\Delta\rho_{min}$ = −1.06 e Å^{-3}

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.

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

	x	y	z	U_{iso}*/U_{eq}
I1	0.65636 (6)	0.37716 (2)	0.58352 (2)	0.02050 (7)
I2	0.65659 (5)	0.36653 (2)	0.30961 (2)	0.01661 (7)
F1	0.1607 (5)	0.17992 (18)	0.21872 (16)	0.0254 (5)
F2	−0.2407 (6)	0.04739 (19)	0.29154 (19)	0.0334 (6)
F3	−0.2418 (6)	0.05622 (19)	0.4886 (2)	0.0326 (6)
F4	0.1622 (6)	0.1944 (2)	0.61205 (17)	0.0280 (6)
C9	0.3758 (8)	0.2652 (3)	0.4798 (3)	0.0154 (7)
C10	0.3778 (8)	0.2613 (3)	0.3784 (3)	0.0151 (7)
C11	0.1718 (9)	0.1857 (3)	0.3168 (3)	0.0174 (8)
C12	−0.0361 (9)	0.1169 (3)	0.3527 (3)	0.0206 (8)
C13	−0.0373 (9)	0.1222 (3)	0.4535 (3)	0.0206 (8)
C14	0.1684 (9)	0.1943 (3)	0.5145 (3)	0.0182 (8)
S1	−0.0441 (2)	0.50172 (8)	0.83086 (7)	0.0204 (2)
N1	0.2256 (7)	0.3842 (3)	0.9578 (2)	0.0184 (7)
HN1	0.165 (10)	0.414 (4)	1.008 (4)	0.029 (13)*
N2	0.2606 (7)	0.3443 (2)	0.8049 (2)	0.0165 (7)
HN2	0.254 (9)	0.349 (3)	0.7436 (15)	0.009 (10)*
C1	0.1504 (9)	0.4093 (3)	0.8658 (3)	0.0186 (8)
C2	0.3863 (8)	0.3038 (3)	0.9558 (3)	0.0172 (8)

C3	0.5098 (9)	0.2511 (3)	1.0292 (3)	0.0215 (8)
H3	0.493986	0.267954	1.096235	0.026*
C4	0.6580 (9)	0.1726 (3)	1.0008 (3)	0.0222 (8)
H4	0.745045	0.135500	1.049815	0.027*
C5	0.6828 (9)	0.1464 (3)	0.9019 (3)	0.0227 (9)
C6	0.5606 (9)	0.2004 (3)	0.8290 (3)	0.0180 (8)
H6	0.578792	0.184847	0.761942	0.022*
C7	0.4108 (9)	0.2782 (3)	0.8579 (3)	0.0176 (8)
C8	0.8415 (9)	0.0590 (3)	0.8758 (3)	0.0245 (9)
H8A	0.727133	−0.005523	0.890936	0.037*
H8B	1.044903	0.071430	0.914124	0.037*
H8C	0.855211	0.054270	0.805416	0.037*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.02224 (14)	0.02260 (14)	0.01557 (12)	0.00692 (10)	−0.00119 (9)	−0.00285 (10)
I2	0.01925 (13)	0.01578 (12)	0.01588 (12)	0.00435 (9)	0.00466 (9)	0.00245 (9)
F1	0.0295 (13)	0.0253 (13)	0.0173 (11)	−0.0002 (10)	−0.0002 (10)	−0.0036 (10)
F2	0.0269 (14)	0.0274 (14)	0.0386 (15)	−0.0070 (11)	−0.0003 (11)	−0.0060 (11)
F3	0.0246 (13)	0.0283 (14)	0.0489 (17)	0.0016 (11)	0.0171 (12)	0.0143 (12)
F4	0.0320 (14)	0.0389 (15)	0.0181 (12)	0.0110 (11)	0.0106 (10)	0.0116 (11)
C9	0.0157 (18)	0.0167 (18)	0.0136 (17)	0.0051 (15)	0.0014 (14)	−0.0022 (14)
C10	0.0173 (18)	0.0148 (18)	0.0135 (17)	0.0033 (14)	0.0024 (14)	0.0016 (14)
C11	0.0205 (19)	0.0172 (19)	0.0151 (18)	0.0071 (15)	0.0012 (14)	0.0000 (15)
C12	0.0161 (19)	0.0167 (19)	0.027 (2)	0.0010 (15)	0.0000 (15)	−0.0015 (16)
C13	0.0132 (18)	0.0170 (19)	0.035 (2)	0.0052 (15)	0.0101 (16)	0.0061 (17)
C14	0.021 (2)	0.021 (2)	0.0155 (18)	0.0099 (16)	0.0041 (15)	0.0056 (15)
S1	0.0227 (5)	0.0197 (5)	0.0214 (5)	0.0062 (4)	0.0081 (4)	0.0052 (4)
N1	0.0228 (18)	0.0185 (17)	0.0150 (16)	0.0047 (14)	0.0065 (13)	0.0005 (13)
N2	0.0214 (17)	0.0202 (17)	0.0102 (15)	0.0073 (13)	0.0045 (12)	0.0037 (13)
C1	0.021 (2)	0.0172 (19)	0.0179 (19)	−0.0010 (15)	0.0066 (15)	0.0044 (15)
C2	0.0175 (19)	0.0193 (19)	0.0152 (18)	0.0014 (15)	0.0063 (14)	0.0018 (15)
C3	0.024 (2)	0.029 (2)	0.0122 (18)	0.0037 (17)	0.0042 (15)	0.0039 (16)
C4	0.020 (2)	0.026 (2)	0.019 (2)	0.0011 (17)	−0.0010 (15)	0.0054 (16)
C5	0.0158 (19)	0.025 (2)	0.026 (2)	0.0015 (16)	0.0018 (16)	0.0020 (17)
C6	0.0193 (19)	0.0207 (19)	0.0145 (18)	0.0041 (16)	0.0039 (15)	0.0014 (15)
C7	0.0192 (19)	0.0186 (19)	0.0146 (18)	0.0027 (15)	0.0023 (14)	0.0018 (15)
C8	0.020 (2)	0.026 (2)	0.029 (2)	0.0066 (17)	0.0019 (17)	0.0049 (18)

Geometric parameters (Å, º)

I1—C9	2.095 (4)	N2—HN2	0.850 (18)
I2—C10	2.106 (4)	N2—C1	1.358 (5)
F1—C11	1.344 (4)	N2—C7	1.393 (5)
F2—C12	1.340 (4)	C2—C3	1.385 (5)
F3—C13	1.340 (4)	C2—C7	1.391 (5)
F4—C14	1.352 (4)	C3—H3	0.9500

C9—C10	1.399 (5)	C3—C4	1.392 (6)
C9—C14	1.383 (5)	C4—H4	0.9500
C10—C11	1.389 (5)	C4—C5	1.406 (6)
C11—C12	1.377 (6)	C5—C6	1.390 (5)
C12—C13	1.389 (6)	C5—C8	1.511 (6)
C13—C14	1.358 (6)	C6—H6	0.9500
S1—C1	1.693 (4)	C6—C7	1.391 (5)
N1—HN1	0.88 (5)	C8—H8A	0.9800
N1—C1	1.351 (5)	C8—H8B	0.9800
N1—C2	1.392 (5)	C8—H8C	0.9800
C10—C9—I1	123.8 (3)	N2—C1—S1	125.9 (3)
C14—C9—I1	117.3 (3)	C3—C2—N1	132.5 (4)
C14—C9—C10	118.8 (3)	C3—C2—C7	120.7 (4)
C9—C10—I2	125.0 (3)	C7—C2—N1	106.9 (3)
C11—C10—I2	116.6 (3)	C2—C3—H3	121.3
C11—C10—C9	118.3 (4)	C2—C3—C4	117.4 (4)
F1—C11—C10	120.6 (3)	C4—C3—H3	121.3
F1—C11—C12	117.3 (3)	C3—C4—H4	119.0
C12—C11—C10	122.0 (4)	C3—C4—C5	122.1 (4)
F2—C12—C11	120.9 (4)	C5—C4—H4	119.0
F2—C12—C13	120.0 (4)	C4—C5—C8	119.4 (4)
C11—C12—C13	119.1 (4)	C6—C5—C4	120.0 (4)
F3—C13—C12	119.2 (4)	C6—C5—C8	120.6 (4)
F3—C13—C14	121.4 (4)	C5—C6—H6	121.2
C14—C13—C12	119.3 (4)	C5—C6—C7	117.5 (4)
F4—C14—C9	120.6 (3)	C7—C6—H6	121.2
F4—C14—C13	116.9 (4)	C2—C7—N2	105.5 (3)
C13—C14—C9	122.5 (4)	C6—C7—N2	132.2 (3)
C1—N1—HN1	121 (3)	C6—C7—C2	122.3 (3)
C1—N1—C2	110.4 (3)	C5—C8—H8A	109.5
C2—N1—HN1	128 (3)	C5—C8—H8B	109.5
C1—N2—HN2	124 (3)	C5—C8—H8C	109.5
C1—N2—C7	111.0 (3)	H8A—C8—H8B	109.5
C7—N2—HN2	125 (3)	H8A—C8—H8C	109.5
N1—C1—S1	127.9 (3)	H8B—C8—H8C	109.5
N1—C1—N2	106.2 (3)		
I1—C9—C10—I2	−0.5 (5)	C14—C9—C10—C11	−0.4 (5)
I1—C9—C10—C11	−177.4 (3)	N1—C2—C3—C4	179.6 (4)
I1—C9—C14—F4	−3.9 (5)	N1—C2—C7—N2	−0.5 (4)
I1—C9—C14—C13	175.8 (3)	N1—C2—C7—C6	179.7 (4)
I2—C10—C11—F1	1.7 (5)	C1—N1—C2—C3	−179.6 (4)
I2—C10—C11—C12	−175.5 (3)	C1—N1—C2—C7	0.0 (4)
F1—C11—C12—F2	−0.1 (5)	C1—N2—C7—C2	0.8 (4)
F1—C11—C12—C13	−178.3 (3)	C1—N2—C7—C6	−179.4 (4)
F2—C12—C13—F3	1.0 (5)	C2—N1—C1—S1	−180.0 (3)
F2—C12—C13—C14	−178.9 (3)	C2—N1—C1—N2	0.5 (4)

F3—C13—C14—F4	1.7 (5)	C2—C3—C4—C5	−0.2 (6)
F3—C13—C14—C9	−178.0 (3)	C3—C2—C7—N2	179.2 (4)
C9—C10—C11—F1	178.8 (3)	C3—C2—C7—C6	−0.7 (6)
C9—C10—C11—C12	1.5 (6)	C3—C4—C5—C6	0.8 (6)
C10—C9—C14—F4	179.0 (3)	C3—C4—C5—C8	−178.8 (4)
C10—C9—C14—C13	−1.3 (6)	C4—C5—C6—C7	−1.3 (6)
C10—C11—C12—F2	177.2 (3)	C5—C6—C7—N2	−178.5 (4)
C10—C11—C12—C13	−1.0 (6)	C5—C6—C7—C2	1.3 (6)
C11—C12—C13—F3	179.2 (3)	C7—N2—C1—S1	179.6 (3)
C11—C12—C13—C14	−0.7 (6)	C7—N2—C1—N1	−0.8 (4)
C12—C13—C14—F4	−178.4 (3)	C7—C2—C3—C4	0.1 (6)
C12—C13—C14—C9	1.9 (6)	C8—C5—C6—C7	178.3 (4)
C14—C9—C10—I2	176.4 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···S1^{i}	0.88 (5)	2.57 (5)	3.444 (3)	173 (4)
N2—H*N*2···I1	0.85 (2)	3.07 (3)	3.780 (3)	142 (3)
N2—H*N*2···F4	0.85 (2)	2.56 (3)	3.122 (4)	124 (3)
C3—H3···I2^{ii}	0.95	3.06	3.966 (4)	160
C6—H6···F4	0.95	2.63	3.262 (4)	125

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

5-Methyl-1*H*-1,3-benzodiazole-2-thiol–1,2,4,5-tetrafluoro-3,6-diiodobenzene–water (2/1/2) (2MMBZIM_14F4DIB_2H2O)

Crystal data

$C_6F_4I_2·2C_8H_8N_2S·2(H_2O)$
M_r = 766.34
Triclinic, $P\overline{1}$
a = 4.9088 (3) Å
b = 11.4670 (8) Å
c = 11.9686 (8) Å
α = 106.644 (2)°
β = 98.058 (2)°
γ = 92.811 (2)°
V = 636.27 (7) Å^3

Z = 1
F(000) = 370
D_x = 2.000 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 9704 reflections
θ = 3.0–29.6°
μ = 2.69 mm^{-1}
T = 100 K
Plate, colourless
0.31 × 0.11 × 0.08 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec I*μ*S
φ and *ω* scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.536, T_{max} = 0.746
31584 measured reflections

3558 independent reflections
3500 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 29.7°, θ_{min} = 3.0°
h = −6→6
k = −15→15
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.014$
$wR(F^2) = 0.034$
$S = 1.18$
3558 reflections
184 parameters
7 restraints

Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + 0.4884P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.44$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
I1	0.44701 (2)	0.37987 (2)	0.76749 (2)	0.01303 (3)	
F1	0.8875 (2)	0.62085 (8)	0.83664 (8)	0.02138 (19)	
F2	1.31349 (19)	0.70566 (8)	1.01073 (9)	0.02069 (19)	
C9	0.7732 (3)	0.45489 (12)	0.90761 (12)	0.0132 (2)	
C10	0.9374 (3)	0.56045 (13)	0.91719 (13)	0.0143 (3)	
C11	1.1591 (3)	0.60420 (12)	1.00759 (13)	0.0145 (3)	
S1	1.03801 (7)	0.78475 (3)	0.43889 (3)	0.01464 (7)	
N1	0.7347 (3)	0.75457 (11)	0.60568 (11)	0.0147 (2)	
HN1	0.770 (4)	0.6828 (15)	0.5977 (19)	0.023 (5)*	
N2	0.7391 (3)	0.93710 (11)	0.58449 (11)	0.0138 (2)	
HN2	0.788 (4)	1.0008 (16)	0.5627 (18)	0.025 (5)*	
C1	0.8342 (3)	0.82603 (13)	0.54519 (12)	0.0136 (2)	
C2	0.5751 (3)	0.82008 (13)	0.68510 (13)	0.0136 (2)	
C3	0.5789 (3)	0.93718 (12)	0.67155 (12)	0.0129 (2)	
C4	0.4354 (3)	1.02719 (13)	0.73639 (13)	0.0154 (3)	
H4	0.437594	1.106246	0.725878	0.018*	
C5	0.2880 (3)	0.99734 (13)	0.81756 (13)	0.0157 (3)	
C6	0.2857 (3)	0.87925 (14)	0.83004 (13)	0.0173 (3)	
H6	0.183714	0.860585	0.885580	0.021*	
C7	0.4267 (3)	0.78842 (14)	0.76427 (14)	0.0176 (3)	
H7	0.421629	0.708673	0.773170	0.021*	
C8	0.1331 (3)	1.09189 (15)	0.89265 (14)	0.0207 (3)	
H8A	−0.041876	1.052972	0.901230	0.031*	
H8B	0.095344	1.155912	0.854696	0.031*	
H8C	0.245015	1.128188	0.970784	0.031*	
O1	0.7691 (3)	0.49501 (11)	0.54916 (12)	0.0247 (2)	
H1AO	0.936 (5)	0.503 (4)	0.532 (4)	0.023 (10)*	0.5
H1BO	0.594 (5)	0.486 (4)	0.516 (4)	0.034 (13)*	0.5
H2O1	0.778 (6)	0.432 (2)	0.575 (3)	0.063 (9)*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01281 (5)	0.01303 (5)	0.01267 (5)	0.00156 (3)	0.00261 (3)	0.00256 (3)
F1	0.0247 (5)	0.0200 (4)	0.0214 (4)	−0.0027 (4)	−0.0034 (4)	0.0133 (4)
F2	0.0216 (4)	0.0163 (4)	0.0242 (5)	−0.0061 (3)	−0.0011 (4)	0.0096 (4)
C9	0.0124 (6)	0.0130 (6)	0.0129 (6)	0.0018 (5)	0.0027 (5)	0.0016 (5)
C10	0.0160 (6)	0.0138 (6)	0.0145 (6)	0.0027 (5)	0.0034 (5)	0.0058 (5)
C11	0.0152 (6)	0.0114 (6)	0.0171 (6)	0.0000 (5)	0.0044 (5)	0.0037 (5)
S1	0.01389 (15)	0.01446 (15)	0.01405 (15)	0.00125 (12)	0.00305 (12)	0.00144 (12)
N1	0.0158 (6)	0.0114 (5)	0.0165 (6)	0.0028 (4)	0.0036 (5)	0.0031 (4)
N2	0.0140 (5)	0.0117 (5)	0.0161 (6)	0.0008 (4)	0.0037 (4)	0.0039 (4)
C1	0.0117 (6)	0.0133 (6)	0.0136 (6)	0.0005 (5)	−0.0006 (5)	0.0021 (5)
C2	0.0126 (6)	0.0123 (6)	0.0156 (6)	0.0012 (5)	0.0011 (5)	0.0042 (5)
C3	0.0112 (6)	0.0125 (6)	0.0138 (6)	−0.0012 (5)	0.0014 (5)	0.0027 (5)
C4	0.0149 (6)	0.0121 (6)	0.0180 (7)	0.0014 (5)	0.0020 (5)	0.0030 (5)
C5	0.0125 (6)	0.0172 (6)	0.0152 (6)	0.0013 (5)	0.0012 (5)	0.0017 (5)
C6	0.0168 (6)	0.0203 (7)	0.0164 (6)	0.0014 (5)	0.0044 (5)	0.0072 (5)
C7	0.0188 (7)	0.0165 (6)	0.0195 (7)	0.0031 (5)	0.0035 (6)	0.0082 (5)
C8	0.0188 (7)	0.0211 (7)	0.0209 (7)	0.0039 (6)	0.0074 (6)	0.0019 (6)
O1	0.0289 (6)	0.0185 (5)	0.0315 (6)	0.0046 (5)	0.0105 (5)	0.0118 (5)

Geometric parameters (Å, º)

I1—C9	2.0981 (14)	C3—C4	1.3888 (19)
F1—C10	1.3424 (16)	C4—H4	0.9500
F2—C11	1.3452 (16)	C4—C5	1.396 (2)
C9—C10	1.3882 (19)	C5—C6	1.404 (2)
C9—C11^{i}	1.386 (2)	C5—C8	1.509 (2)
C10—C11	1.383 (2)	C6—H6	0.9500
S1—C1	1.7035 (15)	C6—C7	1.392 (2)
N1—HN1	0.830 (15)	C7—H7	0.9500
N1—C1	1.3542 (19)	C8—H8A	0.9800
N1—C2	1.3926 (18)	C8—H8B	0.9800
N2—HN2	0.876 (15)	C8—H8C	0.9800
N2—C1	1.3557 (18)	O1—H1AO	0.880 (18)
N2—C3	1.3905 (18)	O1—H1BO	0.883 (18)
C2—C3	1.3975 (19)	O1—H2O1	0.872 (17)
C2—C7	1.387 (2)		
C10—C9—I1	122.63 (11)	C4—C3—N2	131.65 (13)
C11^{i}—C9—I1	120.13 (10)	C4—C3—C2	121.84 (13)
C11^{i}—C9—C10	117.17 (13)	C3—C4—H4	121.2
F1—C10—C9	120.35 (13)	C3—C4—C5	117.61 (13)
F1—C10—C11	118.48 (12)	C5—C4—H4	121.2
C11—C10—C9	121.15 (13)	C4—C5—C6	119.91 (13)
F2—C11—C9^{i}	120.02 (13)	C4—C5—C8	120.20 (14)
F2—C11—C10	118.29 (13)	C6—C5—C8	119.89 (14)

C10—C11—C9^{i}	121.68 (13)	C5—C6—H6	118.7
C1—N1—HN1	124.2 (15)	C7—C6—C5	122.63 (14)
C1—N1—C2	110.28 (12)	C7—C6—H6	118.7
C2—N1—HN1	125.5 (15)	C2—C7—C6	116.72 (14)
C1—N2—HN2	123.8 (14)	C2—C7—H7	121.6
C1—N2—C3	110.09 (12)	C6—C7—H7	121.6
C3—N2—HN2	125.8 (14)	C5—C8—H8A	109.5
N1—C1—S1	126.80 (11)	C5—C8—H8B	109.5
N1—C1—N2	107.02 (12)	C5—C8—H8C	109.5
N2—C1—S1	126.17 (11)	H8A—C8—H8B	109.5
N1—C2—C3	106.11 (12)	H8A—C8—H8C	109.5
C7—C2—N1	132.60 (13)	H8B—C8—H8C	109.5
C7—C2—C3	121.28 (13)	H1AO—O1—H2O1	101 (3)
N2—C3—C2	106.49 (12)	H1BO—O1—H2O1	101 (3)

I1—C9—C10—F1	1.58 (19)	C1—N2—C3—C4	−178.92 (15)
I1—C9—C10—C11	−176.86 (10)	C2—N1—C1—S1	−179.80 (11)
F1—C10—C11—F2	0.3 (2)	C2—N1—C1—N2	−0.27 (16)
F1—C10—C11—C9^{i}	−178.58 (13)	C2—C3—C4—C5	0.7 (2)
C9—C10—C11—F2	178.75 (13)	C3—N2—C1—S1	179.96 (11)
C9—C10—C11—C9^{i}	−0.1 (2)	C3—N2—C1—N1	0.44 (16)
C11^{i}—C9—C10—F1	178.54 (12)	C3—C2—C7—C6	−0.8 (2)
C11^{i}—C9—C10—C11	0.1 (2)	C3—C4—C5—C6	−0.9 (2)
N1—C2—C3—N2	0.25 (15)	C3—C4—C5—C8	178.66 (13)
N1—C2—C3—C4	178.92 (13)	C4—C5—C6—C7	0.2 (2)
N1—C2—C7—C6	−179.24 (15)	C5—C6—C7—C2	0.6 (2)
N2—C3—C4—C5	179.03 (14)	C7—C2—C3—N2	−178.58 (13)
C1—N1—C2—C3	0.01 (16)	C7—C2—C3—C4	0.1 (2)
C1—N1—C2—C7	178.65 (16)	C8—C5—C6—C7	−179.33 (14)
C1—N2—C3—C2	−0.43 (16)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···O1	0.83 (2)	2.06 (2)	2.8763 (17)	166 (2)
N2—H*N*2···S1^{ii}	0.88 (2)	2.57 (2)	3.4211 (13)	164 (2)
C4—H4···I1^{iii}	0.95	3.03	3.9505 (14)	164
O1—H1*AO*···O1^{iv}	0.88 (2)	1.85 (2)	2.708 (3)	163 (4)
O1—H1*BO*···O1^{v}	0.88 (2)	1.89 (2)	2.759 (3)	167 (4)
O1—H2*O*1···I1	0.87 (2)	3.16 (3)	3.7419 (12)	126 (2)
O1—H2*O*1···S1^{iv}	0.87 (2)	2.65 (2)	3.4251 (13)	149 (3)

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

5-Methyl-1*H*-1,3-benzodiazole-2-thiol–1,3,5-trifluoro-2,4,6-\ triiodobenzene (1/1) (MMBZIM_135F3I3B)

Crystal data

$C_6F_3I_3 \cdot C_8H_8N_2S$
$M_r = 673.98$
Monoclinic, $P2_1/c$
$a = 15.191$ (2) Å
$b = 5.0074$ (7) Å
$c = 22.715$ (3) Å
$\beta = 97.460$ (6)°
$V = 1713.3$ (4) Å^3
$Z = 4$
$F(000) = 1232$
$D_x = 2.613$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9964 reflections
$\theta = 2.4$–$27.5°$
$\mu = 5.62$ mm^{-1}
$T = 100$ K
Needle, colourless
0.26 × 0.04 × 0.04 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec IμS
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
$T_{min} = 0.582$, $T_{max} = 0.746$
23258 measured reflections
3971 independent reflections
3039 reflections with $I > 2\sigma(I)$
$R_{int} = 0.069$
$\theta_{max} = 27.6°$, $\theta_{min} = 2.1°$
$h = -19 \rightarrow 19$
$k = -6 \rightarrow 6$
$l = -29 \rightarrow 29$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.105$
$S = 1.22$
3971 reflections
215 parameters
1 restraint
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + 32.9663P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 2.36$ e Å^{-3}
$\Delta\rho_{min} = -1.89$ e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.83468 (4)	0.73539 (12)	0.22592 (3)	0.02269 (15)
I2	1.12973 (3)	0.55191 (11)	0.42927 (2)	0.01871 (14)
I3	0.78829 (3)	−0.06392 (11)	0.42073 (2)	0.01766 (13)
F1	1.0160 (3)	0.7879 (10)	0.3105 (2)	0.0238 (11)
F2	0.9829 (3)	0.1538 (10)	0.4578 (2)	0.0217 (11)
F3	0.7534 (3)	0.2862 (11)	0.3013 (2)	0.0226 (11)
C9	0.8839 (5)	0.5360 (16)	0.3041 (4)	0.0161 (16)
C10	0.9672 (5)	0.5984 (17)	0.3334 (4)	0.0166 (17)
C11	1.0030 (5)	0.4712 (18)	0.3850 (4)	0.0190 (17)
C12	0.9504 (5)	0.2824 (17)	0.4079 (3)	0.0146 (16)

C13	0.8652 (5)	0.2139 (17)	0.3811 (4)	0.0178 (17)
C14	0.8346 (5)	0.3458 (17)	0.3285 (4)	0.0159 (16)
S1	0.34092 (13)	1.4956 (4)	0.50777 (9)	0.0186 (4)
N1	0.4563 (5)	1.2204 (15)	0.4472 (3)	0.0196 (15)
HN1	0.505 (4)	1.302 (17)	0.460 (4)	0.024*
N2	0.3181 (5)	1.1018 (15)	0.4239 (3)	0.0179 (15)
HN2	0.264 (7)	1.10 (2)	0.427 (4)	0.021*
C1	0.3721 (5)	1.2703 (16)	0.4592 (4)	0.0160 (16)
C2	0.4551 (5)	1.0249 (17)	0.4036 (4)	0.0173 (17)
C3	0.5223 (6)	0.9016 (18)	0.3782 (4)	0.0206 (18)
H3	0.582456	0.952312	0.389046	0.025*
C4	0.5000 (5)	0.7020 (17)	0.3364 (4)	0.0204 (18)
C5	0.4109 (6)	0.6252 (18)	0.3226 (4)	0.0212 (18)
H5	0.396802	0.484620	0.294924	0.025*
C6	0.3427 (6)	0.7456 (17)	0.3477 (4)	0.0187 (17)
H6	0.282540	0.695837	0.336564	0.022*
C7	0.3663 (5)	0.9433 (18)	0.3902 (4)	0.0183 (17)
C8	0.5709 (6)	0.561 (2)	0.3080 (4)	0.027 (2)
H8A	0.588556	0.398157	0.330193	0.041*
H8B	0.622521	0.679184	0.308275	0.041*
H8C	0.547999	0.515407	0.266904	0.041*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.0241 (3)	0.0236 (3)	0.0196 (3)	0.0058 (2)	0.0002 (2)	0.0034 (2)
I2	0.0134 (2)	0.0228 (3)	0.0198 (3)	−0.0017 (2)	0.0018 (2)	−0.0022 (2)
I3	0.0150 (2)	0.0183 (3)	0.0204 (3)	−0.0014 (2)	0.0050 (2)	−0.0012 (2)
F1	0.023 (3)	0.026 (3)	0.024 (3)	−0.008 (2)	0.005 (2)	0.007 (2)
F2	0.017 (2)	0.027 (3)	0.019 (3)	0.000 (2)	−0.001 (2)	0.005 (2)
F3	0.012 (2)	0.031 (3)	0.023 (3)	−0.002 (2)	−0.0043 (19)	0.000 (2)
C9	0.017 (4)	0.014 (4)	0.017 (4)	0.003 (3)	0.002 (3)	−0.003 (3)
C10	0.011 (4)	0.022 (4)	0.018 (4)	0.000 (3)	0.006 (3)	0.000 (3)
C11	0.015 (4)	0.024 (5)	0.017 (4)	0.002 (3)	−0.001 (3)	−0.003 (3)
C12	0.014 (4)	0.020 (4)	0.009 (4)	0.001 (3)	0.001 (3)	−0.005 (3)
C13	0.015 (4)	0.021 (4)	0.017 (4)	0.001 (3)	0.003 (3)	0.003 (3)
C14	0.012 (4)	0.018 (4)	0.017 (4)	0.000 (3)	0.001 (3)	−0.002 (3)
S1	0.0153 (9)	0.0217 (11)	0.0185 (10)	−0.0007 (8)	0.0010 (8)	−0.0038 (8)
N1	0.017 (3)	0.018 (4)	0.024 (4)	−0.002 (3)	0.002 (3)	−0.002 (3)
N2	0.010 (3)	0.021 (4)	0.022 (4)	0.001 (3)	0.001 (3)	−0.003 (3)
C1	0.019 (4)	0.010 (4)	0.019 (4)	0.002 (3)	0.002 (3)	0.003 (3)
C2	0.017 (4)	0.018 (4)	0.017 (4)	−0.003 (3)	0.005 (3)	0.010 (3)
C3	0.016 (4)	0.021 (4)	0.026 (5)	−0.003 (3)	0.008 (3)	0.003 (4)
C4	0.016 (4)	0.018 (4)	0.028 (5)	−0.002 (3)	0.003 (3)	−0.010 (4)
C5	0.020 (4)	0.021 (4)	0.023 (5)	−0.006 (3)	0.005 (3)	0.002 (4)
C6	0.017 (4)	0.019 (4)	0.019 (4)	−0.002 (3)	0.001 (3)	0.000 (3)
C7	0.009 (3)	0.026 (5)	0.020 (4)	0.004 (3)	0.000 (3)	−0.001 (4)
C8	0.021 (4)	0.032 (5)	0.030 (5)	0.005 (4)	0.010 (4)	−0.003 (4)

Geometric parameters (Å, º)

I1—C9	2.089 (8)	N2—HN2	0.84 (10)
I2—C11	2.093 (8)	N2—C1	1.363 (11)
I3—C13	2.094 (8)	N2—C7	1.378 (11)
F1—C10	1.349 (9)	C2—C3	1.382 (12)
F2—C12	1.342 (9)	C2—C7	1.405 (11)
F3—C14	1.340 (9)	C3—H3	0.9500
C9—C10	1.388 (11)	C3—C4	1.390 (12)
C9—C14	1.372 (12)	C4—C5	1.402 (11)
C10—C11	1.381 (12)	C4—C8	1.500 (12)
C11—C12	1.382 (12)	C5—H5	0.9500
C12—C13	1.399 (11)	C5—C6	1.384 (12)
C13—C14	1.391 (11)	C6—H6	0.9500
S1—C1	1.688 (8)	C6—C7	1.396 (12)
N1—HN1	0.86 (2)	C8—H8A	0.9800
N1—C1	1.365 (11)	C8—H8B	0.9800
N1—C2	1.391 (11)	C8—H8C	0.9800
C10—C9—I1	120.3 (6)	N2—C1—N1	106.1 (7)
C14—C9—I1	121.5 (6)	N1—C2—C7	106.4 (7)
C14—C9—C10	118.2 (8)	C3—C2—N1	132.1 (8)
F1—C10—C9	119.0 (7)	C3—C2—C7	121.3 (8)
F1—C10—C11	118.5 (7)	C2—C3—H3	120.7
C11—C10—C9	122.5 (8)	C2—C3—C4	118.7 (8)
C10—C11—I2	123.7 (6)	C4—C3—H3	120.7
C10—C11—C12	116.9 (7)	C3—C4—C5	119.4 (8)
C12—C11—I2	119.5 (6)	C3—C4—C8	120.4 (8)
F2—C12—C11	118.6 (7)	C5—C4—C8	120.1 (8)
F2—C12—C13	117.9 (7)	C4—C5—H5	118.6
C11—C12—C13	123.4 (8)	C6—C5—C4	122.8 (8)
C12—C13—I3	120.8 (6)	C6—C5—H5	118.6
C14—C13—I3	122.8 (6)	C5—C6—H6	121.5
C14—C13—C12	116.4 (8)	C5—C6—C7	117.1 (8)
F3—C14—C9	119.0 (7)	C7—C6—H6	121.5
F3—C14—C13	118.4 (7)	N2—C7—C2	106.1 (7)
C9—C14—C13	122.6 (8)	N2—C7—C6	133.3 (7)
C1—N1—HN1	129 (7)	C6—C7—C2	120.6 (8)
C1—N1—C2	110.2 (7)	C4—C8—H8A	109.5
C2—N1—HN1	120 (7)	C4—C8—H8B	109.5
C1—N2—HN2	118 (7)	C4—C8—H8C	109.5
C1—N2—C7	111.2 (7)	H8A—C8—H8B	109.5
C7—N2—HN2	131 (7)	H8A—C8—H8C	109.5
N1—C1—S1	127.0 (6)	H8B—C8—H8C	109.5
N2—C1—S1	126.9 (6)		
I1—C9—C10—F1	−0.4 (10)	C14—C9—C10—C11	1.9 (13)
I1—C9—C10—C11	−179.5 (6)	N1—C2—C3—C4	177.5 (9)

I1—C9—C14—F3	0.4 (11)	N1—C2—C7—N2	2.9 (9)
I1—C9—C14—C13	−178.8 (6)	N1—C2—C7—C6	−179.7 (8)
I2—C11—C12—F2	−0.8 (10)	C1—N1—C2—C3	−177.6 (9)
I2—C11—C12—C13	−179.5 (6)	C1—N1—C2—C7	−2.6 (9)
I3—C13—C14—F3	−2.0 (11)	C1—N2—C7—C2	−2.3 (10)
I3—C13—C14—C9	177.2 (6)	C1—N2—C7—C6	−179.2 (9)
F1—C10—C11—I2	−0.8 (11)	C2—N1—C1—S1	−178.7 (6)
F1—C10—C11—C12	178.6 (7)	C2—N1—C1—N2	1.2 (9)
F2—C12—C13—I3	3.6 (10)	C2—C3—C4—C5	−2.1 (13)
F2—C12—C13—C14	−178.2 (7)	C2—C3—C4—C8	−179.5 (8)
C9—C10—C11—I2	178.3 (6)	C3—C2—C7—N2	178.5 (8)
C9—C10—C11—C12	−2.3 (13)	C3—C2—C7—C6	−4.0 (13)
C10—C9—C14—F3	179.0 (7)	C3—C4—C5—C6	2.0 (14)
C10—C9—C14—C13	−0.2 (13)	C4—C5—C6—C7	−2.7 (13)
C10—C11—C12—F2	179.8 (7)	C5—C6—C7—N2	−179.7 (9)
C10—C11—C12—C13	1.1 (13)	C5—C6—C7—C2	3.7 (13)
C11—C12—C13—I3	−177.6 (6)	C7—N2—C1—S1	−179.4 (6)
C11—C12—C13—C14	0.5 (12)	C7—N2—C1—N1	0.7 (10)
C12—C13—C14—F3	179.9 (7)	C7—C2—C3—C4	3.1 (13)
C12—C13—C14—C9	−0.9 (12)	C8—C4—C5—C6	179.4 (9)
C14—C9—C10—F1	−179.0 (7)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···S1^{i}	0.86 (2)	2.57 (2)	3.427 (7)	174 (9)
N2—H*N*2···I2^{ii}	0.84 (10)	3.03 (10)	3.657 (7)	133 (8)
C3—H3···I3^{iii}	0.95	3.12	4.035 (9)	163
C6—H6···I1^{iv}	0.95	3.14	3.927 (8)	142

Symmetry codes: (i) −*x*+1, −*y*+3, −*z*+1; (ii) *x*−1, *y*+1, *z*; (iii) *x*, *y*+1, *z*; (iv) −*x*+1, *y*−1/2, −*z*+1/2.

1,3-Benzoxazole-2-thiol–1,2,3,4-tetrafluoro-5,6-diiodobenzene (1/1) (MBZOX_12F4DIB)

Crystal data

$C_6F_4I_2·C_7H_5NOS$
M_r = 553.04
Monoclinic, $P2_1/n$
a = 13.7789 (12) Å
b = 4.4129 (4) Å
c = 25.252 (2) Å
β = 96.337 (3)°
V = 1526.0 (2) Å^3
Z = 4
F(000) = 1024
D_x = 2.407 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 5954 reflections
θ = 3.0–26.8°
μ = 4.30 mm^{-1}
T = 100 K
Needle, colourless
0.46 × 0.06 × 0.02 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec I*μ*S
φ and *ω* scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.578, T_{max} = 0.745
12498 measured reflections
3210 independent reflections

2510 reflections with $I > 2\sigma(I)$
$R_{int} = 0.066$
$\theta_{max} = 26.8°$, $\theta_{min} = 3.0°$
$h = -17 \rightarrow 17$
$k = -5 \rightarrow 5$
$l = -31 \rightarrow 31$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.087$
$S = 1.11$
3210 reflections
203 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0191P)^2 + 7.3427P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.58$ e Å^{-3}
$\Delta\rho_{min} = -1.52$ e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.30796 (3)	−0.08467 (10)	0.67864 (2)	0.02151 (14)
I2	0.44314 (3)	−0.05194 (10)	0.81380 (2)	0.01770 (13)
F1	0.6245 (3)	0.3640 (9)	0.80387 (17)	0.0263 (10)
F2	0.6876 (3)	0.6765 (10)	0.7230 (2)	0.0339 (11)
F3	0.5903 (3)	0.6411 (10)	0.62370 (19)	0.0350 (11)
F4	0.4320 (3)	0.2897 (10)	0.60463 (17)	0.0298 (10)
C8	0.4399 (5)	0.1468 (15)	0.6957 (3)	0.0158 (15)
C9	0.4896 (5)	0.1682 (14)	0.7472 (3)	0.0158 (15)
C10	0.5749 (5)	0.3417 (15)	0.7561 (3)	0.0180 (16)
C11	0.6078 (5)	0.4963 (15)	0.7141 (3)	0.0250 (17)
C12	0.5583 (6)	0.4836 (16)	0.6629 (3)	0.0273 (18)
C13	0.4767 (5)	0.3023 (16)	0.6542 (3)	0.0209 (16)
S1	0.07783 (13)	0.0388 (4)	0.57938 (7)	0.0193 (4)
O1	0.2157 (3)	0.4196 (10)	0.55679 (19)	0.0193 (11)
N1	0.1100 (4)	0.3227 (13)	0.4874 (2)	0.0152 (13)
HN1	0.068 (6)	0.228 (18)	0.466 (3)	0.03 (2)*
C1	0.1325 (5)	0.2629 (14)	0.5389 (3)	0.0147 (14)
C2	0.1772 (5)	0.5252 (15)	0.4695 (3)	0.0158 (14)
C3	0.1868 (5)	0.6569 (16)	0.4216 (3)	0.0219 (16)
H3	0.141810	0.617405	0.391053	0.026*
C4	0.2659 (5)	0.8527 (15)	0.4193 (3)	0.0212 (16)
H4	0.274897	0.948201	0.386523	0.025*
C5	0.3316 (6)	0.9111 (16)	0.4637 (3)	0.0229 (16)
H5	0.384448	1.045851	0.460649	0.028*
C6	0.3218 (5)	0.7761 (15)	0.5130 (3)	0.0193 (16)
H6	0.366596	0.813408	0.543631	0.023*
C7	0.2429 (5)	0.5852 (14)	0.5140 (3)	0.0142 (14)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.0210 (3)	0.0213 (2)	0.0210 (3)	−0.0009 (2)	−0.0034 (2)	−0.0037 (2)
I2	0.0223 (2)	0.0177 (2)	0.0130 (2)	0.0024 (2)	0.00165 (18)	−0.00026 (18)
F1	0.018 (2)	0.031 (2)	0.027 (3)	0.0013 (18)	−0.0068 (18)	−0.0058 (19)
F2	0.021 (2)	0.029 (2)	0.052 (3)	−0.0102 (19)	0.010 (2)	−0.003 (2)
F3	0.043 (3)	0.027 (2)	0.039 (3)	−0.001 (2)	0.020 (2)	0.012 (2)
F4	0.041 (3)	0.032 (2)	0.015 (2)	0.005 (2)	−0.001 (2)	0.0042 (19)
C8	0.011 (3)	0.021 (3)	0.016 (4)	0.005 (3)	0.004 (3)	−0.003 (3)
C9	0.016 (3)	0.013 (3)	0.020 (4)	0.005 (3)	0.007 (3)	0.002 (3)
C10	0.016 (4)	0.015 (3)	0.023 (4)	0.004 (3)	−0.001 (3)	−0.006 (3)
C11	0.024 (4)	0.014 (4)	0.038 (5)	0.002 (3)	0.010 (4)	−0.002 (3)
C12	0.037 (5)	0.021 (4)	0.027 (4)	0.005 (3)	0.019 (4)	0.013 (3)
C13	0.027 (4)	0.020 (3)	0.016 (4)	0.010 (3)	0.001 (3)	0.006 (3)
S1	0.0249 (9)	0.0194 (9)	0.0132 (9)	−0.0053 (7)	0.0007 (7)	0.0000 (7)
O1	0.023 (3)	0.017 (2)	0.017 (3)	0.000 (2)	−0.003 (2)	0.003 (2)
N1	0.021 (3)	0.013 (3)	0.010 (3)	0.000 (2)	−0.002 (3)	−0.003 (2)
C1	0.013 (3)	0.012 (3)	0.019 (4)	0.004 (3)	0.003 (3)	−0.002 (3)
C2	0.021 (4)	0.016 (3)	0.011 (4)	0.000 (3)	0.004 (3)	−0.002 (3)
C3	0.026 (4)	0.021 (4)	0.018 (4)	0.000 (3)	0.000 (3)	−0.009 (3)
C4	0.029 (4)	0.016 (3)	0.019 (4)	0.002 (3)	0.005 (3)	0.004 (3)
C5	0.029 (4)	0.018 (4)	0.022 (4)	0.000 (3)	0.008 (3)	0.008 (3)
C6	0.017 (4)	0.018 (4)	0.021 (4)	−0.002 (3)	−0.003 (3)	−0.003 (3)
C7	0.022 (4)	0.012 (3)	0.010 (3)	−0.003 (3)	0.005 (3)	−0.002 (3)

Geometric parameters (Å, º)

I1—C8	2.088 (7)	O1—C7	1.390 (8)
I2—C9	2.101 (7)	N1—HN1	0.85 (8)
F1—C10	1.322 (8)	N1—C1	1.330 (9)
F2—C11	1.355 (8)	N1—C2	1.396 (9)
F3—C12	1.323 (8)	C2—C3	1.364 (10)
F4—C13	1.333 (8)	C2—C7	1.387 (9)
C8—C9	1.406 (10)	C3—H3	0.9500
C8—C13	1.394 (10)	C3—C4	1.397 (10)
C9—C10	1.400 (9)	C4—H4	0.9500
C10—C11	1.380 (11)	C4—C5	1.385 (10)
C11—C12	1.396 (11)	C5—H5	0.9500
C12—C13	1.378 (11)	C5—C6	1.399 (10)
S1—C1	1.662 (7)	C6—H6	0.9500
O1—C1	1.372 (8)	C6—C7	1.378 (9)
C9—C8—I1	123.2 (5)	O1—C1—S1	121.1 (5)
C13—C8—I1	117.8 (5)	N1—C1—S1	130.3 (5)
C13—C8—C9	118.9 (6)	N1—C1—O1	108.6 (6)
C8—C9—I2	123.3 (5)	C3—C2—N1	133.8 (6)
C10—C9—I2	116.7 (5)	C3—C2—C7	121.2 (6)

C10—C9—C8	120.0 (6)	C7—C2—N1	104.9 (6)
F1—C10—C9	121.8 (7)	C2—C3—H3	121.6
F1—C10—C11	118.9 (6)	C2—C3—C4	116.9 (6)
C11—C10—C9	119.3 (7)	C4—C3—H3	121.6
F2—C11—C10	119.5 (7)	C3—C4—H4	119.1
F2—C11—C12	118.9 (7)	C5—C4—C3	121.7 (7)
C10—C11—C12	121.6 (7)	C5—C4—H4	119.1
F3—C12—C11	120.2 (7)	C4—C5—H5	119.3
F3—C12—C13	121.2 (7)	C4—C5—C6	121.4 (7)
C13—C12—C11	118.6 (7)	C6—C5—H5	119.3
F4—C13—C8	121.1 (6)	C5—C6—H6	122.2
F4—C13—C12	117.3 (7)	C7—C6—C5	115.5 (6)
C12—C13—C8	121.5 (7)	C7—C6—H6	122.2
C1—O1—C7	107.2 (5)	C2—C7—O1	108.7 (5)
C1—N1—HN1	126 (6)	C6—C7—O1	128.1 (6)
C1—N1—C2	110.5 (6)	C6—C7—C2	123.2 (6)
C2—N1—HN1	123 (6)		

I1—C8—C9—I2	4.0 (8)	C13—C8—C9—I2	179.9 (5)
I1—C8—C9—C10	−176.3 (5)	C13—C8—C9—C10	−0.5 (10)
I1—C8—C13—F4	−3.7 (9)	N1—C2—C3—C4	−179.9 (7)
I1—C8—C13—C12	173.9 (5)	N1—C2—C7—O1	0.7 (7)
I2—C9—C10—F1	0.7 (8)	N1—C2—C7—C6	179.5 (6)
I2—C9—C10—C11	−178.7 (5)	C1—O1—C7—C2	−1.1 (7)
F1—C10—C11—F2	−2.7 (10)	C1—O1—C7—C6	−180.0 (7)
F1—C10—C11—C12	−179.5 (6)	C1—N1—C2—C3	−179.7 (7)
F2—C11—C12—F3	1.3 (10)	C1—N1—C2—C7	0.1 (7)
F2—C11—C12—C13	−179.3 (6)	C2—N1—C1—S1	−179.8 (5)
F3—C12—C13—F4	0.7 (10)	C2—N1—C1—O1	−0.8 (7)
F3—C12—C13—C8	−177.0 (6)	C2—C3—C4—C5	−0.1 (10)
C8—C9—C10—F1	−179.0 (6)	C3—C2—C7—O1	−179.6 (6)
C8—C9—C10—C11	1.6 (10)	C3—C2—C7—C6	−0.7 (11)
C9—C8—C13—F4	−179.8 (6)	C3—C4—C5—C6	0.1 (11)
C9—C8—C13—C12	−2.2 (10)	C4—C5—C6—C7	−0.4 (10)
C9—C10—C11—F2	176.7 (6)	C5—C6—C7—O1	179.3 (6)
C9—C10—C11—C12	−0.1 (10)	C5—C6—C7—C2	0.7 (10)
C10—C11—C12—F3	178.1 (6)	C7—O1—C1—S1	−179.7 (5)
C10—C11—C12—C13	−2.5 (11)	C7—O1—C1—N1	1.2 (7)
C11—C12—C13—F4	−178.7 (6)	C7—C2—C3—C4	0.3 (10)
C11—C12—C13—C8	3.7 (11)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···S1^{i}	0.85 (8)	2.50 (8)	3.335 (6)	167 (8)
C3—H3···I2^{ii}	0.95	3.19	4.108 (7)	162

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

1,3-Benzoxazole-2-thiol–1,2,3,5-tetrafluoro-4,6-diiodobenzene (1/1) (MBZOX_13F4DIB)

Crystal data

$C_6F_4I_2·C_7H_5NOS$
M_r = 553.04
Monoclinic, $P2_1/c$
a = 15.1655 (8) Å
b = 4.3803 (2) Å
c = 23.0358 (12) Å
β = 99.923 (2)°
V = 1507.36 (13) Å^3
Z = 4
$F(000)$ = 1024
D_x = 2.437 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9330 reflections
θ = 2.7–30.6°
μ = 4.35 mm^{-1}
T = 100 K
Needle, colourless
0.23 × 0.12 × 0.09 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec IμS
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.541, T_{max} = 0.746
39610 measured reflections
4625 independent reflections
4119 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 30.6°, θ_{min} = 2.1°
h = −21→21
k = −6→6
l = −32→32

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.048
S = 1.16
4625 reflections
203 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0088P)^2 + 2.2764P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.96 e Å^{-3}
$\Delta\rho_{min}$ = −1.35 e Å^{-3}

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.

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

	x	y	z	U_{iso}*/U_{eq}
I1	0.71955 (2)	−0.00881 (3)	0.06483 (2)	0.01983 (4)
I2	0.36910 (2)	0.55990 (4)	0.09449 (2)	0.02789 (5)
F1	0.51550 (9)	0.1796 (3)	0.04571 (6)	0.0245 (3)
F2	0.50261 (12)	0.8071 (4)	0.20979 (7)	0.0336 (4)
F3	0.67787 (12)	0.7060 (4)	0.24932 (7)	0.0422 (4)
F4	0.77333 (10)	0.3490 (4)	0.18773 (7)	0.0352 (4)
C8	0.64548 (14)	0.2498 (5)	0.11554 (10)	0.0173 (4)
C9	0.55516 (14)	0.3056 (5)	0.09648 (10)	0.0171 (4)
C10	0.50419 (15)	0.4888 (5)	0.12703 (10)	0.0187 (4)
C11	0.54714 (17)	0.6213 (5)	0.17885 (11)	0.0223 (5)

C12	0.63676 (18)	0.5704 (6)	0.19943 (10)	0.0250 (5)
C13	0.68526 (16)	0.3866 (6)	0.16770 (11)	0.0226 (5)
S1	0.85453 (4)	0.94524 (12)	0.49409 (2)	0.01660 (10)
O1	0.82568 (10)	0.5576 (3)	0.40484 (7)	0.0155 (3)
N1	0.96873 (12)	0.6582 (4)	0.43253 (8)	0.0150 (3)
HN1	1.0171 (19)	0.742 (7)	0.4529 (13)	0.024 (7)*
C1	0.88629 (14)	0.7182 (5)	0.44345 (9)	0.0151 (4)
C2	0.96367 (14)	0.4504 (5)	0.38611 (9)	0.0140 (4)
C3	1.02660 (14)	0.3138 (5)	0.35766 (10)	0.0173 (4)
H3	1.088760	0.354870	0.368581	0.021*
C4	0.99394 (15)	0.1129 (5)	0.31216 (10)	0.0176 (4)
H4	1.035003	0.013545	0.291629	0.021*
C5	0.90240 (15)	0.0533 (5)	0.29583 (10)	0.0182 (4)
H5	0.882849	−0.085313	0.264531	0.022*
C6	0.83913 (14)	0.1930 (5)	0.32450 (10)	0.0177 (4)
H6	0.776786	0.154860	0.313733	0.021*
C7	0.87317 (14)	0.3897 (5)	0.36943 (9)	0.0141 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01738 (7)	0.02028 (7)	0.02311 (8)	0.00339 (5)	0.00709 (5)	0.00604 (5)
I2	0.01897 (8)	0.03084 (9)	0.03563 (10)	0.00756 (6)	0.00974 (6)	0.00672 (7)
F1	0.0175 (6)	0.0307 (8)	0.0242 (7)	−0.0014 (5)	0.0005 (5)	−0.0107 (6)
F2	0.0534 (10)	0.0242 (8)	0.0266 (8)	0.0077 (7)	0.0170 (7)	−0.0037 (6)
F3	0.0559 (11)	0.0436 (10)	0.0218 (8)	−0.0054 (8)	−0.0080 (7)	−0.0099 (7)
F4	0.0236 (7)	0.0491 (10)	0.0282 (8)	0.0008 (7)	−0.0088 (6)	0.0030 (7)
C8	0.0163 (9)	0.0162 (10)	0.0195 (11)	0.0003 (8)	0.0035 (8)	0.0023 (8)
C9	0.0185 (10)	0.0153 (9)	0.0174 (10)	−0.0022 (8)	0.0031 (8)	0.0011 (8)
C10	0.0191 (10)	0.0166 (10)	0.0217 (11)	0.0012 (8)	0.0069 (8)	0.0039 (8)
C11	0.0341 (13)	0.0159 (10)	0.0188 (11)	0.0031 (9)	0.0098 (9)	0.0012 (8)
C12	0.0371 (14)	0.0225 (11)	0.0132 (10)	−0.0046 (10)	−0.0017 (9)	−0.0004 (9)
C13	0.0211 (11)	0.0260 (12)	0.0188 (11)	−0.0016 (9)	−0.0023 (9)	0.0068 (9)
S1	0.0159 (2)	0.0171 (2)	0.0175 (2)	−0.00208 (18)	0.00487 (19)	−0.00332 (19)
O1	0.0127 (7)	0.0170 (7)	0.0166 (7)	−0.0007 (5)	0.0023 (6)	−0.0018 (6)
N1	0.0138 (8)	0.0160 (8)	0.0150 (9)	−0.0025 (6)	0.0022 (6)	−0.0024 (7)
C1	0.0147 (9)	0.0138 (9)	0.0159 (10)	−0.0011 (7)	0.0005 (7)	0.0027 (7)
C2	0.0148 (9)	0.0123 (9)	0.0144 (9)	−0.0004 (7)	0.0015 (7)	0.0013 (7)
C3	0.0149 (9)	0.0189 (10)	0.0184 (10)	0.0007 (8)	0.0037 (8)	0.0027 (8)
C4	0.0205 (10)	0.0166 (10)	0.0166 (10)	0.0019 (8)	0.0059 (8)	0.0020 (8)
C5	0.0228 (10)	0.0173 (10)	0.0147 (10)	−0.0019 (8)	0.0034 (8)	0.0000 (8)
C6	0.0153 (9)	0.0180 (10)	0.0187 (11)	−0.0032 (8)	−0.0005 (8)	−0.0010 (8)
C7	0.0151 (9)	0.0144 (9)	0.0134 (9)	0.0007 (7)	0.0038 (7)	0.0016 (7)

Geometric parameters (Å, º)

I1—C8	2.089 (2)	O1—C7	1.389 (3)
I2—C10	2.080 (2)	N1—HN1	0.88 (3)

F1—C9	1.339 (3)	N1—C1	1.343 (3)
F2—C11	1.339 (3)	N1—C2	1.396 (3)
F3—C12	1.347 (3)	C2—C3	1.383 (3)
F4—C13	1.346 (3)	C2—C7	1.386 (3)
C8—C9	1.386 (3)	C3—H3	0.9500
C8—C13	1.384 (3)	C3—C4	1.393 (3)
C9—C10	1.387 (3)	C4—H4	0.9500
C10—C11	1.385 (3)	C4—C5	1.399 (3)
C11—C12	1.378 (4)	C5—H5	0.9500
C12—C13	1.382 (4)	C5—C6	1.396 (3)
S1—C1	1.666 (2)	C6—H6	0.9500
O1—C1	1.360 (2)	C6—C7	1.377 (3)

C9—C8—I1	121.04 (17)	O1—C1—S1	121.49 (15)
C13—C8—I1	121.61 (17)	N1—C1—S1	129.70 (17)
C13—C8—C9	117.2 (2)	N1—C1—O1	108.82 (18)
F1—C9—C8	118.4 (2)	C3—C2—N1	133.9 (2)
F1—C9—C10	118.4 (2)	C3—C2—C7	121.1 (2)
C8—C9—C10	123.2 (2)	C7—C2—N1	104.99 (18)
C9—C10—I2	120.27 (17)	C2—C3—H3	121.8
C11—C10—I2	122.39 (17)	C2—C3—C4	116.4 (2)
C11—C10—C9	117.3 (2)	C4—C3—H3	121.8
F2—C11—C10	120.5 (2)	C3—C4—H4	119.1
F2—C11—C12	118.2 (2)	C3—C4—C5	121.9 (2)
C12—C11—C10	121.2 (2)	C5—C4—H4	119.1
F3—C12—C11	120.4 (2)	C4—C5—H5	119.3
F3—C12—C13	119.9 (2)	C6—C5—C4	121.5 (2)
C11—C12—C13	119.7 (2)	C6—C5—H5	119.3
F4—C13—C8	120.2 (2)	C5—C6—H6	122.2
F4—C13—C12	118.5 (2)	C7—C6—C5	115.5 (2)
C12—C13—C8	121.3 (2)	C7—C6—H6	122.2
C1—O1—C7	107.32 (16)	C2—C7—O1	108.94 (18)
C1—N1—HN1	122.5 (19)	C6—C7—O1	127.43 (19)
C1—N1—C2	109.92 (18)	C6—C7—C2	123.6 (2)
C2—N1—HN1	127.6 (19)		

I1—C8—C9—F1	2.6 (3)	C13—C8—C9—F1	179.0 (2)
I1—C8—C9—C10	−176.56 (17)	C13—C8—C9—C10	−0.1 (3)
I1—C8—C13—F4	−1.6 (3)	N1—C2—C3—C4	179.9 (2)
I1—C8—C13—C12	176.58 (18)	N1—C2—C7—O1	0.2 (2)
I2—C10—C11—F2	−1.1 (3)	N1—C2—C7—C6	−180.0 (2)
I2—C10—C11—C12	180.00 (18)	C1—O1—C7—C2	−0.6 (2)
F1—C9—C10—I2	0.6 (3)	C1—O1—C7—C6	179.6 (2)
F1—C9—C10—C11	−178.8 (2)	C1—N1—C2—C3	−179.9 (2)
F2—C11—C12—F3	−0.2 (3)	C1—N1—C2—C7	0.3 (2)
F2—C11—C12—C13	−178.2 (2)	C2—N1—C1—S1	179.30 (17)
F3—C12—C13—F4	−0.3 (4)	C2—N1—C1—O1	−0.7 (2)
F3—C12—C13—C8	−178.4 (2)	C2—C3—C4—C5	0.3 (3)

C8—C9—C10—I2	179.72 (17)	C3—C2—C7—O1	−179.62 (19)
C8—C9—C10—C11	0.3 (3)	C3—C2—C7—C6	0.2 (3)
C9—C8—C13—F4	−178.0 (2)	C3—C4—C5—C6	0.0 (3)
C9—C8—C13—C12	0.1 (3)	C4—C5—C6—C7	−0.2 (3)
C9—C10—C11—F2	178.3 (2)	C5—C6—C7—O1	179.9 (2)
C9—C10—C11—C12	−0.6 (3)	C5—C6—C7—C2	0.1 (3)
C10—C11—C12—F3	178.7 (2)	C7—O1—C1—S1	−179.20 (15)
C10—C11—C12—C13	0.7 (4)	C7—O1—C1—N1	0.8 (2)
C11—C12—C13—F4	177.8 (2)	C7—C2—C3—C4	−0.4 (3)
C11—C12—C13—C8	−0.4 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···S1^{i}	0.88 (3)	2.52 (3)	3.3906 (19)	172 (3)
C3—H3···I1^{ii}	0.95	3.10	4.030 (2)	166

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

1,3-Benzoxazole-2-thiol–1,2,4,5-tetrafluoro-3,6-diiodobenzene (2/1) (2MBZOX_14F4DIB)

Crystal data

$C_6F_4I_2·2C_7H_5NOS$
M_r = 704.22
Monoclinic, *C*2/*c*
a = 31.025 (4) Å
b = 4.3159 (5) Å
c = 19.061 (2) Å
β = 114.434 (4)°
V = 2323.6 (5) Å^3
Z = 4
F(000) = 1336
D_x = 2.013 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 9971 reflections
θ = 2.4–28.7°
μ = 2.94 mm^{-1}
T = 100 K
Tabular, colourless
0.29 × 0.12 × 0.03 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec I*μ*S
φ and *ω* scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.637, T_{max} = 0.746
25197 measured reflections
2950 independent reflections
2571 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 28.7°, θ_{min} = 2.2°
h = −41→41
k = −5→5
l = −25→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.060
S = 1.32
2950 reflections
149 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + 11.7646P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 1.54 e Å^{-3}
$\Delta\rho_{min}$ = −1.15 e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.64136 (2)	0.39079 (5)	0.46092 (2)	0.01937 (7)
F1	0.71102 (7)	0.7954 (5)	0.60381 (11)	0.0276 (5)
F2	0.70741 (7)	0.4164 (5)	0.36823 (11)	0.0273 (5)
C8	0.70659 (11)	0.6029 (8)	0.48500 (19)	0.0189 (6)
C9	0.72975 (11)	0.7707 (8)	0.55172 (19)	0.0194 (7)
C10	0.72770 (12)	0.5825 (8)	0.43364 (19)	0.0201 (7)
S1	0.54594 (3)	0.0194 (2)	0.43700 (5)	0.01964 (17)
O1	0.49241 (8)	0.4059 (5)	0.32770 (12)	0.0181 (5)
N1	0.46292 (10)	0.3062 (7)	0.41195 (16)	0.0180 (6)
HN1	0.4609 (14)	0.224 (10)	0.452 (2)	0.028 (11)*
C1	0.49912 (12)	0.2491 (8)	0.39283 (18)	0.0182 (6)
C2	0.43102 (12)	0.5092 (8)	0.35848 (18)	0.0187 (6)
C3	0.38827 (12)	0.6362 (8)	0.35038 (19)	0.0227 (7)
H3	0.374567	0.592471	0.385578	0.027*
C4	0.36660 (12)	0.8320 (8)	0.2875 (2)	0.0253 (7)
H4	0.337264	0.925746	0.279739	0.030*
C5	0.38649 (13)	0.8950 (8)	0.2355 (2)	0.0251 (7)
H5	0.370406	1.030939	0.193581	0.030*
C6	0.42930 (12)	0.7643 (8)	0.24340 (19)	0.0224 (7)
H6	0.443055	0.805267	0.208135	0.027*
C7	0.45026 (11)	0.5714 (7)	0.30592 (18)	0.0181 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01700 (11)	0.01887 (11)	0.02288 (11)	−0.00041 (8)	0.00889 (8)	0.00070 (8)
F1	0.0248 (10)	0.0379 (12)	0.0253 (10)	−0.0054 (9)	0.0154 (9)	−0.0045 (9)
F2	0.0246 (10)	0.0342 (12)	0.0238 (10)	−0.0064 (9)	0.0107 (9)	−0.0095 (9)
C8	0.0180 (15)	0.0161 (15)	0.0231 (16)	−0.0009 (12)	0.0092 (13)	0.0014 (13)
C9	0.0178 (15)	0.0229 (17)	0.0198 (16)	0.0016 (13)	0.0101 (13)	0.0002 (13)
C10	0.0196 (16)	0.0197 (16)	0.0190 (15)	0.0010 (13)	0.0061 (13)	−0.0027 (13)
S1	0.0185 (4)	0.0201 (4)	0.0209 (4)	−0.0009 (3)	0.0089 (3)	0.0015 (3)
O1	0.0198 (11)	0.0198 (12)	0.0159 (10)	−0.0014 (9)	0.0087 (9)	0.0002 (9)
N1	0.0202 (14)	0.0190 (14)	0.0166 (13)	0.0002 (11)	0.0092 (11)	0.0030 (11)
C1	0.0217 (16)	0.0163 (16)	0.0172 (15)	−0.0055 (13)	0.0085 (13)	−0.0038 (12)
C2	0.0239 (17)	0.0140 (15)	0.0164 (15)	−0.0035 (13)	0.0064 (13)	−0.0009 (12)
C3	0.0219 (16)	0.0246 (18)	0.0220 (16)	0.0004 (14)	0.0094 (14)	−0.0018 (14)
C4	0.0212 (17)	0.0241 (19)	0.0289 (18)	−0.0004 (14)	0.0088 (15)	−0.0016 (15)
C5	0.0274 (18)	0.0215 (17)	0.0206 (16)	−0.0003 (15)	0.0041 (14)	0.0016 (14)

C6	0.0274 (18)	0.0226 (18)	0.0174 (16)	−0.0048 (14)	0.0097 (14)	0.0001 (13)
C7	0.0185 (15)	0.0158 (16)	0.0194 (15)	−0.0034 (12)	0.0073 (13)	−0.0026 (12)

Geometric parameters (Å, º)

I1—C8	2.092 (3)	N1—C2	1.397 (4)
F1—C9	1.346 (4)	C2—C3	1.383 (5)
F2—C10	1.347 (4)	C2—C7	1.388 (4)
C8—C9	1.379 (5)	C3—H3	0.9500
C8—C10	1.388 (4)	C3—C4	1.391 (5)
C9—C10^{i}	1.385 (5)	C4—H4	0.9500
S1—C1	1.670 (3)	C4—C5	1.393 (5)
O1—C1	1.352 (4)	C5—H5	0.9500
O1—C7	1.394 (4)	C5—C6	1.393 (5)
N1—HN1	0.87 (4)	C6—H6	0.9500
N1—C1	1.339 (4)	C6—C7	1.376 (5)
C9—C8—I1	121.3 (2)	C3—C2—C7	121.4 (3)
C9—C8—C10	117.8 (3)	C7—C2—N1	105.2 (3)
C10—C8—I1	120.9 (2)	C2—C3—H3	122.1
F1—C9—C8	120.2 (3)	C2—C3—C4	115.9 (3)
F1—C9—C10^{i}	118.8 (3)	C4—C3—H3	122.1
C8—C9—C10^{i}	121.1 (3)	C3—C4—H4	118.9
F2—C10—C8	120.7 (3)	C3—C4—C5	122.2 (3)
F2—C10—C9^{i}	118.1 (3)	C5—C4—H4	118.9
C9^{i}—C10—C8	121.2 (3)	C4—C5—H5	119.1
C1—O1—C7	107.4 (2)	C6—C5—C4	121.8 (3)
C1—N1—HN1	123 (3)	C6—C5—H5	119.1
C1—N1—C2	109.7 (3)	C5—C6—H6	122.4
C2—N1—HN1	128 (3)	C7—C6—C5	115.2 (3)
O1—C1—S1	122.1 (2)	C7—C6—H6	122.4
N1—C1—S1	128.6 (3)	C2—C7—O1	108.5 (3)
N1—C1—O1	109.2 (3)	C6—C7—O1	128.1 (3)
C3—C2—N1	133.4 (3)	C6—C7—C2	123.5 (3)
I1—C8—C9—F1	1.5 (4)	C1—N1—C2—C7	−0.1 (4)
I1—C8—C9—C10^{i}	−178.3 (3)	C2—N1—C1—S1	−179.1 (3)
I1—C8—C10—F2	−2.3 (4)	C2—N1—C1—O1	−0.4 (4)
I1—C8—C10—C9^{i}	178.3 (3)	C2—C3—C4—C5	0.4 (5)
C9—C8—C10—F2	178.5 (3)	C3—C2—C7—O1	−178.4 (3)
C9—C8—C10—C9^{i}	−0.9 (6)	C3—C2—C7—C6	1.1 (5)
C10—C8—C9—F1	−179.4 (3)	C3—C4—C5—C6	0.3 (6)
C10—C8—C9—C10^{i}	0.9 (6)	C4—C5—C6—C7	−0.3 (5)
N1—C2—C3—C4	−179.6 (3)	C5—C6—C7—O1	179.0 (3)
N1—C2—C7—O1	0.5 (3)	C5—C6—C7—C2	−0.4 (5)
N1—C2—C7—C6	180.0 (3)	C7—O1—C1—S1	179.5 (2)
C1—O1—C7—C2	−0.8 (3)	C7—O1—C1—N1	0.8 (3)

C1—O1—C7—C6	179.8 (3)	C7—C2—C3—C4	−1.0 (5)
C1—N1—C2—C3	178.6 (4)		

Symmetry code: (i) −*x*+3/2, −*y*+3/2, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···S1^{ii}	0.87 (4)	2.45 (4)	3.316 (3)	178 (4)
C3—H3···I1^{iii}	0.95	3.16	4.066 (3)	159

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

1,3-Benzoxazole-2-thiol–1,3,5-trifluoro-2,4,6-triiodobenzene (1/1) (MBZOX_135F3I3B)

Crystal data

$C_6F_3I_3·C_7H_5NOS$
M_r = 660.94
Monoclinic, $P2_1/c$
a = 14.9295 (7) Å
b = 4.6119 (2) Å
c = 23.5065 (12) Å
β = 92.548 (2)°
V = 1616.90 (13) Å^3
Z = 4
$F(000)$ = 1200
D_x = 2.715 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9982 reflections
θ = 2.7–26.5°
μ = 5.96 mm^{-1}
T = 100 K
Column, colourless
0.22 × 0.06 × 0.05 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec IμS
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.551, T_{max} = 0.745
19413 measured reflections
3348 independent reflections
2845 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 26.6°, θ_{min} = 2.2°
h = −18→18
k = −5→5
l = −29→29

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.061
S = 1.22
3348 reflections
203 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0015P)^2 + 8.0148P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.80 e Å^{-3}
$\Delta\rho_{min}$ = −0.77 e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.70807 (2)	0.45232 (7)	0.55419 (2)	0.01748 (9)
I2	0.67869 (2)	1.23515 (8)	0.76030 (2)	0.02173 (10)
I3	0.36351 (2)	1.08539 (8)	0.59175 (2)	0.02080 (10)
F1	0.75694 (18)	0.8001 (7)	0.66897 (14)	0.0224 (7)
F2	0.4884 (2)	1.2983 (7)	0.69902 (14)	0.0233 (7)
F3	0.50893 (19)	0.6840 (7)	0.54104 (13)	0.0216 (7)
C8	0.6336 (3)	0.7273 (11)	0.6051 (2)	0.0148 (10)
C9	0.6700 (3)	0.8566 (12)	0.6536 (2)	0.0171 (11)
C10	0.6230 (3)	1.0473 (12)	0.6861 (2)	0.0172 (11)
C11	0.5357 (3)	1.1100 (11)	0.6684 (2)	0.0182 (11)
C12	0.4950 (3)	0.9888 (12)	0.6197 (2)	0.0161 (11)
C13	0.5456 (3)	0.8001 (11)	0.5888 (2)	0.0150 (11)
S1	0.85264 (8)	0.0073 (3)	0.48739 (6)	0.0189 (3)
O1	0.8417 (2)	0.3886 (8)	0.40283 (15)	0.0173 (8)
N1	0.9806 (3)	0.3173 (10)	0.43450 (19)	0.0160 (9)
HN1	1.021 (4)	0.235 (15)	0.456 (3)	0.04 (2)*
C1	0.8953 (3)	0.2405 (12)	0.4417 (2)	0.0179 (11)
C2	0.9850 (3)	0.5192 (11)	0.3901 (2)	0.0161 (11)
C3	1.0549 (4)	0.6679 (12)	0.3661 (2)	0.0214 (12)
H3	1.115554	0.640591	0.378875	0.026*
C4	1.0309 (4)	0.8596 (12)	0.3222 (2)	0.0209 (12)
H4	1.076369	0.965301	0.304220	0.025*
C5	0.9402 (4)	0.9002 (12)	0.3038 (2)	0.0215 (12)
H5	0.926165	1.034052	0.274018	0.026*
C6	0.8718 (3)	0.7504 (12)	0.3281 (2)	0.0194 (11)
H6	0.810884	0.774932	0.315558	0.023*
C7	0.8969 (3)	0.5632 (11)	0.3715 (2)	0.0175 (11)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01571 (16)	0.01825 (18)	0.01870 (18)	0.00147 (13)	0.00332 (13)	0.00178 (14)
I2	0.02249 (18)	0.0226 (2)	0.01963 (19)	−0.00506 (14)	−0.00417 (14)	−0.00151 (15)
I3	0.01328 (16)	0.0296 (2)	0.01939 (19)	0.00433 (14)	−0.00095 (13)	0.00351 (16)
F1	0.0106 (14)	0.0263 (18)	0.0298 (18)	0.0009 (12)	−0.0040 (13)	0.0000 (15)
F2	0.0196 (15)	0.0230 (18)	0.0274 (18)	0.0043 (13)	0.0018 (13)	−0.0061 (15)
F3	0.0164 (15)	0.0279 (18)	0.0201 (16)	0.0002 (13)	−0.0031 (12)	−0.0072 (14)
C8	0.019 (3)	0.006 (2)	0.018 (3)	0.0031 (19)	−0.004 (2)	−0.002 (2)
C9	0.010 (2)	0.021 (3)	0.020 (3)	−0.001 (2)	0.001 (2)	0.007 (2)
C10	0.015 (2)	0.024 (3)	0.012 (3)	−0.003 (2)	0.000 (2)	0.001 (2)
C11	0.018 (3)	0.011 (3)	0.026 (3)	0.001 (2)	0.007 (2)	0.003 (2)
C12	0.011 (2)	0.020 (3)	0.017 (3)	−0.001 (2)	−0.001 (2)	0.002 (2)
C13	0.015 (2)	0.015 (3)	0.014 (3)	−0.0009 (19)	−0.002 (2)	0.001 (2)
S1	0.0167 (6)	0.0202 (7)	0.0200 (7)	0.0025 (5)	0.0036 (5)	0.0035 (6)
O1	0.0153 (17)	0.019 (2)	0.0177 (19)	0.0016 (14)	0.0007 (14)	0.0059 (16)

N1	0.012 (2)	0.023 (3)	0.012 (2)	0.0051 (18)	−0.0012 (17)	0.0016 (19)
C1	0.016 (2)	0.022 (3)	0.016 (3)	0.006 (2)	−0.002 (2)	−0.005 (2)
C2	0.014 (2)	0.015 (3)	0.018 (3)	0.004 (2)	−0.001 (2)	−0.004 (2)
C3	0.018 (3)	0.025 (3)	0.021 (3)	0.002 (2)	0.002 (2)	−0.001 (2)
C4	0.023 (3)	0.020 (3)	0.020 (3)	−0.002 (2)	0.011 (2)	−0.002 (2)
C5	0.037 (3)	0.017 (3)	0.011 (3)	0.004 (2)	0.003 (2)	0.002 (2)
C6	0.016 (3)	0.021 (3)	0.021 (3)	0.005 (2)	−0.002 (2)	−0.002 (2)
C7	0.018 (3)	0.014 (3)	0.020 (3)	−0.001 (2)	0.002 (2)	−0.004 (2)

Geometric parameters (Å, º)

I1—C8	2.096 (5)	O1—C7	1.387 (6)
I2—C10	2.086 (5)	N1—HN1	0.85 (7)
I3—C12	2.091 (5)	N1—C1	1.340 (7)
F1—C9	1.356 (5)	N1—C2	1.403 (7)
F2—C11	1.347 (6)	C2—C3	1.389 (8)
F3—C13	1.340 (6)	C2—C7	1.383 (7)
C8—C9	1.378 (7)	C3—H3	0.9500
C8—C13	1.392 (7)	C3—C4	1.393 (8)
C9—C10	1.378 (8)	C4—H4	0.9500
C10—C11	1.381 (7)	C4—C5	1.415 (8)
C11—C12	1.389 (7)	C5—H5	0.9500
C12—C13	1.379 (7)	C5—C6	1.377 (8)
S1—C1	1.666 (6)	C6—H6	0.9500
O1—C1	1.370 (6)	C6—C7	1.376 (8)
C9—C8—I1	122.3 (4)	O1—C1—S1	121.6 (4)
C9—C8—C13	117.1 (5)	N1—C1—S1	130.2 (4)
C13—C8—I1	120.5 (4)	N1—C1—O1	108.3 (5)
F1—C9—C8	118.4 (5)	C3—C2—N1	133.7 (5)
F1—C9—C10	118.7 (5)	C7—C2—N1	104.9 (4)
C10—C9—C8	122.9 (5)	C7—C2—C3	121.4 (5)
C9—C10—I2	122.3 (4)	C2—C3—H3	121.9
C9—C10—C11	117.7 (5)	C2—C3—C4	116.2 (5)
C11—C10—I2	120.0 (4)	C4—C3—H3	121.9
F2—C11—C10	119.0 (5)	C3—C4—H4	119.3
F2—C11—C12	118.7 (5)	C3—C4—C5	121.4 (5)
C10—C11—C12	122.4 (5)	C5—C4—H4	119.3
C11—C12—I3	122.9 (4)	C4—C5—H5	119.2
C13—C12—I3	119.8 (4)	C6—C5—C4	121.6 (5)
C13—C12—C11	117.3 (5)	C6—C5—H5	119.2
F3—C13—C8	118.6 (4)	C5—C6—H6	122.0
F3—C13—C12	118.7 (4)	C7—C6—C5	116.1 (5)
C12—C13—C8	122.7 (5)	C7—C6—H6	122.0
C1—O1—C7	107.6 (4)	C2—C7—O1	109.0 (5)
C1—N1—HN1	117 (5)	C6—C7—O1	127.6 (5)
C1—N1—C2	110.2 (4)	C6—C7—C2	123.4 (5)
C2—N1—HN1	132 (5)		

I1—C8—C9—F1	−0.7 (7)	C13—C8—C9—F1	−177.0 (5)
I1—C8—C9—C10	177.2 (4)	C13—C8—C9—C10	0.9 (8)
I1—C8—C13—F3	2.0 (7)	N1—C2—C3—C4	−178.6 (5)
I1—C8—C13—C12	−177.5 (4)	N1—C2—C7—O1	−1.3 (6)
I2—C10—C11—F2	1.5 (7)	N1—C2—C7—C6	179.5 (5)
I2—C10—C11—C12	−179.3 (4)	C1—O1—C7—C2	1.3 (6)
I3—C12—C13—F3	0.4 (7)	C1—O1—C7—C6	−179.6 (5)
I3—C12—C13—C8	179.9 (4)	C1—N1—C2—C3	179.1 (6)
F1—C9—C10—I2	−3.2 (7)	C1—N1—C2—C7	0.9 (6)
F1—C9—C10—C11	177.6 (5)	C2—N1—C1—S1	179.1 (4)
F2—C11—C12—I3	−0.1 (7)	C2—N1—C1—O1	−0.2 (6)
F2—C11—C12—C13	179.1 (5)	C2—C3—C4—C5	0.5 (8)
C8—C9—C10—I2	178.9 (4)	C3—C2—C7—O1	−179.7 (5)
C8—C9—C10—C11	−0.3 (8)	C3—C2—C7—C6	1.0 (8)
C9—C8—C13—F3	178.3 (5)	C3—C4—C5—C6	−0.6 (8)
C9—C8—C13—C12	−1.1 (8)	C4—C5—C6—C7	0.8 (8)
C9—C10—C11—F2	−179.2 (5)	C5—C6—C7—O1	179.9 (5)
C9—C10—C11—C12	−0.1 (8)	C5—C6—C7—C2	−1.1 (8)
C10—C11—C12—I3	−179.2 (4)	C7—O1—C1—S1	180.0 (4)
C10—C11—C12—C13	−0.1 (8)	C7—O1—C1—N1	−0.7 (6)
C11—C12—C13—F3	−178.7 (5)	C7—C2—C3—C4	−0.7 (8)
C11—C12—C13—C8	0.7 (8)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···S1^{i}	0.85 (7)	2.53 (7)	3.377 (4)	176 (6)
C3—H3···I1^{ii}	0.95	3.04	3.969 (5)	167
C6—H6···I2^{iii}	0.95	3.23	4.009 (5)	140

Symmetry codes: (i) −*x*+2, −*y*, −*z*+1; (ii) −*x*+2, −*y*+1, −*z*+1; (iii) *x*, −*y*+5/2, *z*−1/2.

1,3-Benzothiazole-2-thiol)–1,2,3,4-tetrafluoro-5,6-diiodobenzene (3/4) (3MBZTH_412F4DIB)

Crystal data

$4C_6F_4I_2·3C_7H_5NS_2$
M_r = 2109.16
Triclinic, $P\overline{1}$
a = 7.9410 (8) Å
b = 14.8483 (15) Å
c = 24.641 (3) Å
α = 79.264 (4)°
β = 87.104 (4)°
γ = 82.784 (4)°
V = 2830.9 (5) Å^3
Z = 2
F(000) = 1940
D_x = 2.474 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
μ = 4.69 mm^{-1}
T = 100 K
Plate, colourless
0.30 × 0.13 × 0.04 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec I*μ*S
φ and *ω* scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.570, T_{max} = 0.746
78566 measured reflections

12466 independent reflections
11325 reflections with $I > 2\sigma(I)$
$R_{int} = 0.067$
$\theta_{max} = 27.2°$, $\theta_{min} = 2.5°$
$h = -10 \rightarrow 10$
$k = -19 \rightarrow 19$
$l = -31 \rightarrow 31$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.067$
$wR(F^2) = 0.220$
$S = 1.06$
12466 reflections
704 parameters
66 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1285P)^2 + 109.2112P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 2.61$ e Å^{-3}
$\Delta\rho_{min} = -1.48$ e Å^{-3}

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. Refined as a 2-component twin.

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

	x	y	z	U_{iso}*/U_{eq}
I1	0.36226 (13)	1.16753 (7)	0.05962 (4)	0.0199 (2)
I2	−0.11193 (13)	1.17703 (7)	0.07045 (4)	0.0192 (2)
S3	0.8569 (5)	0.2851 (3)	0.27854 (18)	0.0222 (8)
S4	0.9358 (5)	0.3501 (3)	0.15807 (18)	0.0219 (8)
F1	−0.1901 (12)	0.9764 (7)	0.0748 (4)	0.023 (2)
F2	0.0046 (12)	0.8143 (6)	0.0705 (4)	0.0210 (18)
F3	0.3454 (12)	0.8083 (6)	0.0614 (4)	0.0218 (19)
F4	0.4959 (11)	0.9599 (7)	0.0585 (4)	0.023 (2)
N2	0.7575 (18)	0.4523 (10)	0.2157 (6)	0.022 (3)
HN2	0.702118	0.472763	0.243675	0.026*
C8	0.8414 (19)	0.3657 (12)	0.2214 (7)	0.022 (3)
C9	0.8613 (18)	0.4590 (11)	0.1256 (8)	0.022 (3)
C10	0.877 (2)	0.5034 (12)	0.0712 (7)	0.025 (3)
H10	0.946102	0.474610	0.045108	0.030*
C11	0.792 (3)	0.5893 (13)	0.0558 (8)	0.033 (3)
H11	0.792908	0.617175	0.017859	0.040*
C12	0.704 (2)	0.6375 (13)	0.0933 (8)	0.029 (3)
H12	0.656903	0.699744	0.081256	0.035*
C13	0.683 (2)	0.5975 (11)	0.1470 (8)	0.024 (3)
H13	0.616999	0.629053	0.172475	0.029*
C14	0.764 (2)	0.5071 (12)	0.1632 (7)	0.021 (3)
C22	0.2314 (19)	1.0522 (10)	0.0647 (6)	0.014 (3)
C23	0.0557 (18)	1.0544 (10)	0.0689 (6)	0.016 (3)
C24	−0.0213 (17)	0.9775 (10)	0.0714 (6)	0.014 (2)
C25	0.0758 (19)	0.8923 (10)	0.0684 (6)	0.015 (2)

C26	0.2483 (19)	0.8892 (10)	0.0642 (6)	0.016 (3)
C27	0.3254 (18)	0.9675 (10)	0.0619 (6)	0.015 (3)
I3	0.64678 (12)	1.13261 (7)	0.23166 (4)	0.0194 (2)
I4	0.18439 (13)	1.10869 (8)	0.23135 (5)	0.0227 (2)
F5	0.1660 (12)	0.9119 (8)	0.2046 (5)	0.028 (2)
F6	0.4004 (14)	0.7773 (7)	0.1803 (5)	0.032 (2)
F7	0.7341 (13)	0.8013 (7)	0.1742 (5)	0.028 (2)
F8	0.8342 (12)	0.9554 (7)	0.1967 (5)	0.027 (2)
C28	0.548 (2)	1.0190 (11)	0.2120 (6)	0.019 (3)
C29	0.3765 (17)	1.0068 (10)	0.2139 (6)	0.014 (3)
C30	0.3304 (19)	0.9261 (12)	0.2037 (6)	0.019 (3)
C31	0.447 (2)	0.8555 (11)	0.1910 (7)	0.020 (3)
C32	0.618 (2)	0.8672 (12)	0.1869 (7)	0.022 (3)
C33	0.6663 (18)	0.9461 (11)	0.1986 (7)	0.018 (3)
I5	0.23233 (12)	0.71859 (7)	0.32850 (4)	0.0183 (2)
I6	−0.23322 (12)	0.70593 (7)	0.32425 (4)	0.0200 (2)
F9	−0.4093 (13)	0.8951 (8)	0.3451 (4)	0.028 (2)
F10	−0.2991 (13)	1.0414 (7)	0.3748 (5)	0.028 (2)
F11	0.0385 (13)	1.0534 (7)	0.3782 (5)	0.027 (2)
F12	0.2640 (12)	0.9152 (7)	0.3547 (5)	0.026 (2)
C34	0.0485 (19)	0.8268 (10)	0.3394 (6)	0.017 (3)
C35	−0.1293 (18)	0.8223 (10)	0.3377 (6)	0.015 (2)
C36	−0.2433 (18)	0.8975 (10)	0.3469 (6)	0.016 (2)
C37	−0.1897 (18)	0.9730 (10)	0.3622 (6)	0.015 (2)
C38	−0.016 (2)	0.9776 (11)	0.3644 (7)	0.020 (3)
C39	0.097 (2)	0.9065 (10)	0.3535 (7)	0.019 (3)
I7	0.02233 (13)	0.46575 (7)	0.37019 (4)	0.0196 (2)
I8	−0.02757 (15)	0.35978 (8)	0.51719 (5)	0.0269 (3)
F13	0.1440 (16)	0.1570 (8)	0.5289 (4)	0.036 (3)
F14	0.3307 (17)	0.0627 (7)	0.4593 (5)	0.037 (3)
F15	0.3867 (14)	0.1426 (7)	0.3536 (4)	0.030 (2)
F16	0.2600 (13)	0.3180 (7)	0.3159 (4)	0.026 (2)
C40	0.1256 (19)	0.3310 (9)	0.4037 (6)	0.015 (3)
C41	0.100 (2)	0.2902 (12)	0.4582 (7)	0.020 (3)
C42	0.171 (2)	0.2029 (13)	0.4767 (7)	0.025 (3)
C43	0.263 (2)	0.1486 (12)	0.4419 (7)	0.023 (3)
C44	0.292 (2)	0.1890 (11)	0.3876 (7)	0.022 (3)
C45	0.223 (2)	0.2791 (10)	0.3680 (6)	0.017 (3)
S1	0.5243 (5)	0.5375 (3)	0.31454 (16)	0.0193 (7)
S2	0.4491 (5)	0.4693 (3)	0.43557 (17)	0.0217 (8)
N1	0.6185 (17)	0.3686 (9)	0.3737 (6)	0.020 (2)
HN1	0.671175	0.349037	0.345043	0.025*
C1	0.5386 (19)	0.4543 (10)	0.3712 (6)	0.0156 (18)
C2	0.518 (2)	0.3547 (12)	0.4654 (7)	0.022 (3)
C3	0.498 (2)	0.3107 (13)	0.5198 (6)	0.024 (3)
H3	0.442344	0.342280	0.547045	0.029*
C4	0.566 (3)	0.2171 (16)	0.5328 (9)	0.042 (5)
H4	0.548501	0.183201	0.568902	0.050*

C5	0.659 (3)	0.1730 (14)	0.4927 (8)	0.037 (5)
H5	0.705227	0.110313	0.502792	0.044*
C6	0.684 (2)	0.2196 (12)	0.4377 (8)	0.028 (4)
H6	0.746640	0.190247	0.410614	0.033*
C7	0.610 (2)	0.3135 (11)	0.4259 (8)	0.024 (3)
S5	0.5779 (5)	0.3528 (3)	0.04223 (16)	0.0185 (7)
S6	0.4242 (5)	0.3654 (3)	0.15534 (16)	0.0196 (7)
N3	0.3879 (16)	0.4977 (9)	0.0733 (5)	0.016 (2)
HN3	0.397601	0.531273	0.040138	0.019*
C15	0.4623 (19)	0.4112 (10)	0.0858 (6)	0.016 (3)
C16	0.3061 (19)	0.4678 (10)	0.1659 (6)	0.016 (3)
C17	0.216 (2)	0.4894 (11)	0.2134 (6)	0.021 (3)
H17	0.215714	0.445412	0.246790	0.025*
C18	0.128 (2)	0.5768 (12)	0.2101 (7)	0.025 (3)
H18	0.074519	0.594232	0.242502	0.030*
C19	0.116 (2)	0.6408 (11)	0.1597 (8)	0.026 (4)
H19	0.048383	0.698679	0.158241	0.032*
C20	0.2008 (19)	0.6197 (10)	0.1133 (7)	0.019 (3)
H20	0.197834	0.663313	0.079745	0.022*
C21	0.2922 (19)	0.5323 (10)	0.1166 (6)	0.015 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.0179 (5)	0.0178 (5)	0.0249 (5)	−0.0061 (4)	0.0017 (4)	−0.0046 (4)
I2	0.0168 (5)	0.0176 (4)	0.0238 (5)	0.0017 (3)	0.0003 (4)	−0.0076 (4)
S3	0.026 (2)	0.0144 (17)	0.026 (2)	0.0011 (14)	0.0023 (16)	−0.0064 (15)
S4	0.0223 (19)	0.0171 (18)	0.027 (2)	−0.0012 (14)	0.0041 (16)	−0.0092 (15)
F1	0.014 (4)	0.025 (5)	0.030 (5)	−0.001 (4)	0.001 (4)	−0.004 (4)
F2	0.021 (2)	0.022 (2)	0.022 (2)	−0.0089 (18)	−0.0027 (18)	−0.0044 (18)
F3	0.016 (4)	0.016 (4)	0.032 (5)	0.004 (3)	0.000 (4)	−0.006 (4)
F4	0.007 (4)	0.024 (5)	0.038 (6)	−0.004 (3)	0.001 (4)	−0.006 (4)
N2	0.020 (7)	0.020 (7)	0.026 (7)	0.002 (5)	0.001 (5)	−0.009 (6)
C8	0.011 (7)	0.025 (8)	0.032 (9)	−0.002 (6)	−0.011 (6)	−0.011 (7)
C9	0.004 (6)	0.021 (8)	0.043 (10)	0.000 (5)	−0.001 (6)	−0.011 (7)
C10	0.030 (7)	0.021 (7)	0.025 (7)	0.001 (6)	−0.012 (6)	−0.009 (6)
C11	0.042 (7)	0.028 (7)	0.031 (7)	0.011 (6)	−0.019 (6)	−0.013 (6)
C12	0.028 (7)	0.025 (7)	0.034 (7)	0.002 (6)	−0.010 (6)	−0.008 (6)
C13	0.012 (7)	0.019 (8)	0.041 (10)	−0.001 (6)	−0.005 (7)	−0.007 (7)
C14	0.023 (8)	0.024 (8)	0.019 (7)	−0.009 (6)	0.015 (6)	−0.010 (6)
C22	0.018 (7)	0.014 (6)	0.006 (6)	0.004 (5)	0.001 (5)	0.001 (5)
C23	0.009 (5)	0.018 (6)	0.018 (6)	0.001 (5)	0.002 (5)	−0.001 (5)
C24	0.005 (5)	0.016 (5)	0.021 (5)	0.002 (4)	0.004 (4)	−0.004 (4)
C25	0.016 (6)	0.013 (6)	0.016 (6)	0.000 (5)	0.002 (5)	−0.004 (5)
C26	0.016 (7)	0.015 (7)	0.017 (7)	0.006 (5)	−0.008 (6)	−0.008 (6)
C27	0.012 (6)	0.012 (6)	0.020 (7)	0.001 (5)	0.004 (5)	−0.005 (6)
I3	0.0164 (5)	0.0180 (5)	0.0230 (5)	−0.0020 (3)	0.0015 (4)	−0.0025 (4)
I4	0.0135 (4)	0.0257 (5)	0.0256 (5)	0.0039 (4)	0.0016 (4)	−0.0007 (4)

F5	0.010 (4)	0.041 (6)	0.036 (6)	−0.007 (4)	0.001 (4)	−0.012 (5)
F6	0.026 (5)	0.025 (5)	0.049 (7)	−0.004 (4)	−0.003 (5)	−0.013 (5)
F7	0.022 (5)	0.028 (5)	0.036 (6)	0.000 (4)	0.004 (4)	−0.015 (4)
F8	0.009 (4)	0.028 (5)	0.047 (6)	−0.003 (4)	0.001 (4)	−0.013 (5)
C28	0.019 (8)	0.017 (7)	0.016 (7)	0.001 (6)	0.008 (6)	0.001 (6)
C29	0.006 (6)	0.018 (7)	0.022 (7)	−0.003 (5)	−0.001 (5)	−0.010 (6)
C30	0.013 (7)	0.034 (9)	0.008 (6)	−0.003 (6)	−0.005 (5)	−0.001 (6)
C31	0.016 (7)	0.020 (7)	0.025 (8)	0.000 (6)	−0.005 (6)	−0.004 (6)
C32	0.020 (8)	0.027 (8)	0.021 (8)	−0.001 (6)	−0.004 (6)	−0.007 (6)
C33	0.004 (6)	0.022 (8)	0.028 (8)	−0.002 (5)	0.003 (6)	−0.007 (6)
I5	0.0127 (4)	0.0181 (4)	0.0233 (5)	0.0019 (3)	0.0022 (4)	−0.0047 (4)
I6	0.0161 (5)	0.0194 (5)	0.0249 (5)	−0.0025 (4)	−0.0033 (4)	−0.0039 (4)
F9	0.016 (5)	0.031 (5)	0.032 (5)	0.002 (4)	−0.001 (4)	0.004 (4)
F10	0.022 (5)	0.020 (5)	0.042 (6)	0.008 (4)	0.002 (4)	−0.010 (4)
F11	0.025 (5)	0.022 (5)	0.038 (6)	−0.004 (4)	−0.001 (4)	−0.013 (4)
F12	0.012 (4)	0.020 (5)	0.043 (6)	−0.002 (4)	−0.001 (4)	0.003 (4)
C34	0.014 (7)	0.008 (6)	0.023 (7)	0.003 (5)	0.003 (6)	0.007 (5)
C35	0.008 (5)	0.016 (5)	0.020 (5)	−0.001 (4)	−0.003 (4)	0.004 (4)
C36	0.006 (4)	0.017 (5)	0.020 (5)	0.001 (4)	−0.001 (4)	0.004 (4)
C37	0.006 (5)	0.017 (5)	0.021 (5)	0.001 (4)	0.001 (4)	0.001 (4)
C38	0.021 (8)	0.017 (7)	0.021 (7)	−0.001 (6)	−0.004 (6)	0.003 (6)
C39	0.027 (8)	0.010 (6)	0.019 (7)	−0.004 (6)	0.001 (6)	0.000 (5)
I7	0.0181 (5)	0.0162 (4)	0.0234 (5)	0.0003 (3)	−0.0028 (4)	−0.0016 (4)
I8	0.0288 (6)	0.0313 (6)	0.0212 (5)	−0.0007 (4)	0.0039 (4)	−0.0091 (4)
F13	0.048 (7)	0.029 (6)	0.022 (5)	−0.004 (5)	0.001 (5)	0.012 (4)
F14	0.056 (8)	0.018 (5)	0.033 (6)	0.009 (5)	−0.011 (5)	0.000 (4)
F15	0.031 (6)	0.030 (5)	0.030 (5)	0.010 (4)	0.007 (4)	−0.016 (4)
F16	0.026 (5)	0.030 (5)	0.018 (5)	0.003 (4)	0.006 (4)	0.001 (4)
C40	0.019 (7)	0.007 (6)	0.017 (7)	0.003 (5)	0.002 (5)	−0.002 (5)
C41	0.015 (6)	0.027 (7)	0.017 (6)	−0.002 (5)	−0.006 (5)	0.003 (5)
C42	0.019 (6)	0.035 (7)	0.013 (5)	0.009 (5)	0.001 (5)	0.007 (5)
C43	0.022 (6)	0.022 (7)	0.020 (6)	0.004 (6)	−0.008 (5)	0.004 (5)
C44	0.024 (8)	0.020 (8)	0.024 (8)	−0.002 (6)	0.002 (6)	−0.009 (6)
C45	0.018 (7)	0.014 (7)	0.016 (7)	0.003 (5)	0.002 (6)	0.000 (6)
S1	0.0186 (17)	0.0161 (17)	0.0224 (18)	0.0004 (14)	0.0010 (14)	−0.0038 (14)
S2	0.0197 (18)	0.0264 (19)	0.0195 (17)	0.0001 (15)	0.0006 (14)	−0.0077 (15)
N1	0.020 (5)	0.021 (5)	0.023 (5)	−0.004 (4)	−0.001 (4)	−0.007 (4)
C1	0.015 (4)	0.019 (4)	0.017 (4)	−0.006 (3)	−0.002 (3)	−0.010 (3)
C2	0.015 (7)	0.030 (9)	0.021 (8)	−0.008 (6)	0.003 (6)	−0.003 (7)
C3	0.019 (8)	0.042 (10)	0.010 (7)	−0.005 (7)	0.001 (6)	−0.001 (7)
C4	0.041 (12)	0.051 (13)	0.032 (10)	−0.030 (10)	−0.007 (9)	0.011 (9)
C5	0.058 (13)	0.026 (9)	0.022 (9)	−0.008 (9)	−0.008 (8)	0.010 (7)
C6	0.031 (9)	0.018 (8)	0.033 (9)	−0.004 (7)	−0.012 (7)	0.001 (7)
C7	0.026 (8)	0.014 (7)	0.031 (9)	−0.002 (6)	−0.009 (7)	0.002 (6)
S5	0.0195 (18)	0.0119 (16)	0.0226 (18)	0.0032 (13)	0.0020 (14)	−0.0028 (14)
S6	0.0213 (18)	0.0154 (17)	0.0201 (18)	0.0013 (14)	−0.0005 (14)	−0.0005 (14)
N3	0.016 (6)	0.014 (6)	0.017 (6)	0.004 (5)	0.000 (5)	−0.003 (5)
C15	0.018 (7)	0.011 (6)	0.020 (7)	−0.002 (5)	−0.007 (6)	−0.001 (5)

C16	0.013 (7)	0.015 (7)	0.019 (7)	−0.001 (5)	0.002 (5)	−0.002 (6)
C17	0.031 (9)	0.021 (8)	0.009 (6)	0.001 (7)	−0.003 (6)	0.002 (6)
C18	0.016 (7)	0.030 (9)	0.028 (8)	0.004 (6)	0.001 (6)	−0.009 (7)
C19	0.033 (9)	0.012 (7)	0.033 (9)	0.007 (6)	−0.006 (7)	−0.008 (7)
C20	0.016 (7)	0.014 (7)	0.024 (8)	−0.005 (6)	0.013 (6)	0.000 (6)
C21	0.018 (7)	0.012 (6)	0.016 (7)	−0.005 (5)	0.004 (5)	−0.004 (5)

Geometric parameters (Å, º)

I1—C22	2.094 (15)	C35—C36	1.39 (2)
I2—C23	2.121 (15)	C36—C37	1.37 (2)
S3—C8	1.669 (18)	C37—C38	1.40 (2)
S4—C8	1.738 (18)	C38—C39	1.35 (2)
S4—C9	1.711 (17)	I7—C40	2.097 (14)
F1—C24	1.341 (16)	I8—C41	2.086 (17)
F2—C25	1.344 (17)	F13—C42	1.358 (19)
F3—C26	1.355 (16)	F14—C43	1.320 (19)
F4—C27	1.344 (17)	F15—C44	1.328 (18)
N2—HN2	0.8800	F16—C45	1.341 (18)
N2—C8	1.36 (2)	C40—C41	1.38 (2)
N2—C14	1.40 (2)	C40—C45	1.41 (2)
C9—C10	1.39 (3)	C41—C42	1.35 (2)
C9—C14	1.42 (2)	C42—C43	1.40 (2)
C10—H10	0.9500	C43—C44	1.38 (2)
C10—C11	1.36 (2)	C44—C45	1.39 (2)
C11—H11	0.9500	S1—C1	1.680 (16)
C11—C12	1.38 (3)	S2—C1	1.747 (15)
C12—H12	0.9500	S2—C2	1.755 (19)
C12—C13	1.36 (3)	N1—HN1	0.8800
C13—H13	0.9500	N1—C1	1.34 (2)
C13—C14	1.41 (2)	N1—C7	1.39 (2)
C22—C23	1.39 (2)	C2—C3	1.39 (2)
C22—C27	1.391 (19)	C2—C7	1.38 (2)
C23—C24	1.35 (2)	C3—H3	0.9500
C24—C25	1.408 (19)	C3—C4	1.41 (3)
C25—C26	1.36 (2)	C4—H4	0.9500
C26—C27	1.37 (2)	C4—C5	1.41 (3)
I3—C28	2.089 (16)	C5—H5	0.9500
I4—C29	2.097 (14)	C5—C6	1.42 (3)
F5—C30	1.347 (18)	C6—H6	0.9500
F6—C31	1.336 (19)	C6—C7	1.43 (2)
F7—C32	1.330 (19)	S5—C15	1.671 (16)
F8—C33	1.355 (17)	S6—C15	1.749 (16)
C28—C29	1.40 (2)	S6—C16	1.740 (15)
C28—C33	1.42 (2)	N3—HN3	0.8800
C29—C30	1.37 (2)	N3—C15	1.331 (19)
C30—C31	1.38 (2)	N3—C21	1.416 (19)
C31—C32	1.38 (2)	C16—C17	1.41 (2)

C32—C33	1.36 (2)	C16—C21	1.40 (2)
I5—C34	2.077 (14)	C17—H17	0.9500
I6—C35	2.092 (15)	C17—C18	1.38 (2)
F9—C36	1.326 (17)	C18—H18	0.9500
F10—C37	1.323 (17)	C18—C19	1.41 (3)
F11—C38	1.359 (19)	C19—H19	0.9500
F12—C39	1.348 (19)	C19—C20	1.36 (2)
C34—C35	1.43 (2)	C20—H20	0.9500
C34—C39	1.40 (2)	C20—C21	1.40 (2)

C9—S4—C8	93.5 (8)	C39—C38—F11	120.7 (15)
C8—N2—HN2	121.8	C39—C38—C37	120.0 (15)
C8—N2—C14	116.5 (14)	F12—C39—C34	119.1 (14)
C14—N2—HN2	121.8	F12—C39—C38	117.8 (14)
S3—C8—S4	123.8 (10)	C38—C39—C34	123.1 (16)
N2—C8—S3	127.4 (14)	C41—C40—I7	123.4 (11)
N2—C8—S4	108.8 (13)	C41—C40—C45	118.8 (14)
C10—C9—S4	131.6 (13)	C45—C40—I7	117.7 (11)
C10—C9—C14	118.2 (15)	C40—C41—I8	123.5 (12)
C14—C9—S4	110.2 (14)	C42—C41—I8	116.4 (12)
C9—C10—H10	120.7	C42—C41—C40	119.9 (15)
C11—C10—C9	118.6 (17)	F13—C42—C43	114.0 (15)
C11—C10—H10	120.7	C41—C42—F13	123.0 (15)
C10—C11—H11	118.7	C41—C42—C43	122.7 (15)
C10—C11—C12	122.6 (19)	F14—C43—C42	123.2 (15)
C12—C11—H11	118.7	F14—C43—C44	118.8 (16)
C11—C12—H12	119.4	C44—C43—C42	117.9 (15)
C13—C12—C11	121.1 (18)	F15—C44—C43	120.7 (15)
C13—C12—H12	119.4	F15—C44—C45	119.1 (15)
C12—C13—H13	121.5	C43—C44—C45	120.3 (15)
C12—C13—C14	116.9 (16)	F16—C45—C40	120.7 (13)
C14—C13—H13	121.5	F16—C45—C44	118.9 (14)
N2—C14—C9	111.1 (15)	C44—C45—C40	120.3 (14)
N2—C14—C13	126.8 (15)	C1—S2—C2	92.1 (8)
C13—C14—C9	122.1 (16)	C1—N1—HN1	123.1
C23—C22—I1	124.6 (10)	C1—N1—C7	113.8 (14)
C23—C22—C27	117.2 (14)	C7—N1—HN1	123.1
C27—C22—I1	118.1 (11)	S1—C1—S2	123.6 (9)
C22—C23—I2	123.4 (11)	N1—C1—S1	125.7 (12)
C24—C23—I2	114.8 (10)	N1—C1—S2	110.7 (12)
C24—C23—C22	121.8 (14)	C3—C2—S2	128.6 (14)
F1—C24—C23	123.9 (13)	C7—C2—S2	108.1 (12)
F1—C24—C25	115.8 (13)	C7—C2—C3	123.1 (17)
C23—C24—C25	120.3 (13)	C2—C3—H3	121.6
F2—C25—C24	122.3 (13)	C2—C3—C4	116.9 (17)
F2—C25—C26	119.2 (13)	C4—C3—H3	121.6
C26—C25—C24	118.5 (13)	C3—C4—H4	119.6
F3—C26—C25	120.0 (13)	C3—C4—C5	120.8 (17)

F3—C26—C27	119.2 (13)	C5—C4—H4	119.6
C25—C26—C27	120.8 (13)	C4—C5—H5	119.0
F4—C27—C22	120.4 (13)	C4—C5—C6	122.0 (19)
F4—C27—C26	118.2 (13)	C6—C5—H5	119.0
C26—C27—C22	121.4 (14)	C5—C6—H6	122.2
C29—C28—I3	125.4 (11)	C5—C6—C7	115.5 (18)
C29—C28—C33	117.2 (14)	C7—C6—H6	122.2
C33—C28—I3	117.3 (11)	N1—C7—C6	123.2 (17)
C28—C29—I4	122.4 (11)	C2—C7—N1	115.2 (15)
C30—C29—I4	118.3 (10)	C2—C7—C6	121.5 (17)
C30—C29—C28	119.3 (14)	C16—S6—C15	91.6 (7)
F5—C30—C29	121.1 (14)	C15—N3—HN3	122.0
F5—C30—C31	116.1 (15)	C15—N3—C21	116.0 (13)
C29—C30—C31	122.7 (14)	C21—N3—HN3	122.0
F6—C31—C30	122.3 (14)	S5—C15—S6	123.6 (9)
F6—C31—C32	118.6 (15)	N3—C15—S5	125.8 (12)
C30—C31—C32	119.1 (15)	N3—C15—S6	110.6 (12)
F7—C32—C31	121.1 (15)	C17—C16—S6	129.9 (12)
F7—C32—C33	119.9 (14)	C21—C16—S6	110.9 (11)
C33—C32—C31	119.0 (15)	C21—C16—C17	118.9 (14)
F8—C33—C28	118.8 (14)	C16—C17—H17	121.0
F8—C33—C32	118.6 (14)	C18—C17—C16	117.9 (15)
C32—C33—C28	122.6 (14)	C18—C17—H17	121.0
C35—C34—I5	123.6 (11)	C17—C18—H18	119.0
C39—C34—I5	119.6 (11)	C17—C18—C19	121.9 (15)
C39—C34—C35	116.6 (14)	C19—C18—H18	119.0
C34—C35—I6	123.6 (11)	C18—C19—H19	119.9
C36—C35—I6	116.8 (10)	C20—C19—C18	120.3 (15)
C36—C35—C34	119.6 (14)	C20—C19—H19	119.9
F9—C36—C35	120.7 (14)	C19—C20—H20	121.0
F9—C36—C37	117.6 (13)	C19—C20—C21	118.0 (15)
C37—C36—C35	121.5 (13)	C21—C20—H20	121.0
F10—C37—C36	121.4 (13)	C16—C21—N3	110.8 (13)
F10—C37—C38	119.6 (14)	C20—C21—N3	126.5 (14)
C36—C37—C38	119.0 (14)	C20—C21—C16	122.6 (14)
F11—C38—C37	119.3 (14)		

I1—C22—C23—I2	0.4 (18)	F11—C38—C39—F12	−3 (2)
I1—C22—C23—C24	179.1 (11)	F11—C38—C39—C34	179.7 (14)
I1—C22—C27—F4	2.9 (19)	C34—C35—C36—F9	179.6 (14)
I1—C22—C27—C26	−179.1 (11)	C34—C35—C36—C37	−6 (2)
I2—C23—C24—F1	0 (2)	C35—C34—C39—F12	−178.7 (13)
I2—C23—C24—C25	177.4 (11)	C35—C34—C39—C38	−1 (2)
S4—C9—C10—C11	174.9 (14)	C35—C36—C37—F10	−175.0 (14)
S4—C9—C14—N2	0.4 (17)	C35—C36—C37—C38	5 (2)
S4—C9—C14—C13	−178.2 (13)	C36—C37—C38—F11	178.3 (14)
F1—C24—C25—F2	−2 (2)	C36—C37—C38—C39	−3 (2)
F1—C24—C25—C26	179.3 (13)	C37—C38—C39—F12	178.2 (14)

F2—C25—C26—F3	1 (2)	C37—C38—C39—C34	1 (2)
F2—C25—C26—C27	179.9 (13)	C39—C34—C35—I6	−174.6 (11)
F3—C26—C27—F4	−2 (2)	C39—C34—C35—C36	3 (2)
F3—C26—C27—C22	−179.9 (13)	I7—C40—C41—I8	−5.3 (19)
C8—S4—C9—C10	−178.3 (16)	I7—C40—C41—C42	179.9 (13)
C8—S4—C9—C14	−0.2 (12)	I7—C40—C45—F16	6 (2)
C8—N2—C14—C9	−1 (2)	I7—C40—C45—C44	−178.8 (12)
C8—N2—C14—C13	178.0 (16)	I8—C41—C42—F13	8 (2)
C9—S4—C8—S3	−179.6 (10)	I8—C41—C42—C43	−178.7 (14)
C9—S4—C8—N2	−0.1 (12)	F13—C42—C43—F14	−5 (3)
C9—C10—C11—C12	6 (3)	F13—C42—C43—C44	178.0 (15)
C10—C9—C14—N2	178.8 (14)	F14—C43—C44—F15	−1 (3)
C10—C9—C14—C13	0 (2)	F14—C43—C44—C45	−179.9 (15)
C10—C11—C12—C13	−7 (3)	F15—C44—C45—F16	−3 (2)
C11—C12—C13—C14	4 (3)	F15—C44—C45—C40	−178.3 (15)
C12—C13—C14—N2	−178.8 (16)	C40—C41—C42—F13	−176.5 (16)
C12—C13—C14—C9	0 (2)	C40—C41—C42—C43	−4 (3)
C14—N2—C8—S3	179.9 (12)	C41—C40—C45—F16	−175.7 (14)
C14—N2—C8—S4	0.4 (17)	C41—C40—C45—C44	0 (2)
C14—C9—C10—C11	−3 (2)	C41—C42—C43—F14	−178.9 (17)
C22—C23—C24—F1	−179.2 (14)	C41—C42—C43—C44	4 (3)
C22—C23—C24—C25	−1 (2)	C42—C43—C44—F15	176.2 (16)
C23—C22—C27—F4	−179.1 (13)	C42—C43—C44—C45	−3 (3)
C23—C22—C27—C26	−1 (2)	C43—C44—C45—F16	176.8 (15)
C23—C24—C25—F2	−179.8 (14)	C43—C44—C45—C40	1 (2)
C23—C24—C25—C26	1 (2)	C45—C40—C41—I8	176.1 (11)
C24—C25—C26—F3	179.9 (13)	C45—C40—C41—C42	1 (2)
C24—C25—C26—C27	−1 (2)	S2—C2—C3—C4	179.7 (14)
C25—C26—C27—F4	179.1 (14)	S2—C2—C7—N1	−3.3 (18)
C25—C26—C27—C22	1 (2)	S2—C2—C7—C6	179.8 (14)
C27—C22—C23—I2	−177.4 (11)	C1—S2—C2—C3	178.1 (16)
C27—C22—C23—C24	1 (2)	C1—S2—C2—C7	2.8 (13)
I3—C28—C29—I4	5.1 (19)	C1—N1—C7—C2	2 (2)
I3—C28—C29—C30	−175.4 (11)	C1—N1—C7—C6	179.0 (15)
I3—C28—C33—F8	−3 (2)	C2—S2—C1—S1	178.3 (10)
I3—C28—C33—C32	177.7 (13)	C2—S2—C1—N1	−1.8 (12)
I4—C29—C30—F5	0 (2)	C2—C3—C4—C5	4 (3)
I4—C29—C30—C31	179.0 (12)	C3—C2—C7—N1	−178.9 (15)
F5—C30—C31—F6	0 (2)	C3—C2—C7—C6	4 (3)
F5—C30—C31—C32	177.2 (14)	C3—C4—C5—C6	−2 (3)
F6—C31—C32—F7	−2 (2)	C4—C5—C6—C7	0 (3)
F6—C31—C32—C33	−179.0 (15)	C5—C6—C7—N1	−177.9 (17)
F7—C32—C33—F8	0 (2)	C5—C6—C7—C2	−1 (3)
F7—C32—C33—C28	179.6 (15)	C7—N1—C1—S1	−179.9 (12)
C28—C29—C30—F5	−179.4 (14)	C7—N1—C1—S2	0.2 (16)
C28—C29—C30—C31	0 (2)	C7—C2—C3—C4	−6 (3)
C29—C28—C33—F8	−179.5 (14)	S6—C16—C17—C18	−178.4 (13)
C29—C28—C33—C32	1 (2)	S6—C16—C21—N3	−4.0 (16)

C29—C30—C31—F6	−179.1 (15)	S6—C16—C21—C20	178.7 (12)
C29—C30—C31—C32	−2 (2)	C15—S6—C16—C17	176.4 (16)
C30—C31—C32—F7	−179.3 (15)	C15—S6—C16—C21	2.5 (12)
C30—C31—C32—C33	4 (2)	C15—N3—C21—C16	4.0 (19)
C31—C32—C33—F8	177.3 (15)	C15—N3—C21—C20	−178.8 (15)
C31—C32—C33—C28	−3 (3)	C16—S6—C15—S5	179.3 (10)
C33—C28—C29—I4	−178.6 (11)	C16—S6—C15—N3	−0.3 (12)
C33—C28—C29—C30	1 (2)	C16—C17—C18—C19	5 (3)
I5—C34—C35—I6	0.3 (19)	C17—C16—C21—N3	−178.6 (14)
I5—C34—C35—C36	178.4 (11)	C17—C16—C21—C20	4 (2)
I5—C34—C39—F12	6 (2)	C17—C18—C19—C20	−4 (3)
I5—C34—C39—C38	−176.1 (12)	C18—C19—C20—C21	3 (3)
I6—C35—C36—F9	−2.2 (19)	C19—C20—C21—N3	−180.0 (15)
I6—C35—C36—C37	172.5 (12)	C19—C20—C21—C16	−3 (2)
F9—C36—C37—F10	0 (2)	C21—N3—C15—S5	178.4 (11)
F9—C36—C37—C38	−179.9 (14)	C21—N3—C15—S6	−2.0 (17)
F10—C37—C38—F11	−1 (2)	C21—C16—C17—C18	−5 (2)
F10—C37—C38—C39	177.6 (15)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H*N*2···S1	0.88	2.45	3.326 (14)	174
N1—H*N*1···S3	0.88	2.40	3.266 (14)	169
C6—H6···F10^{i}	0.95	2.60	3.29 (2)	130
N3—H*N*3···S5^{ii}	0.88	2.42	3.290 (14)	170
C17—H17···F16	0.95	2.30	3.232 (18)	166
C20—H20···F2	0.95	2.53	3.128 (18)	121
C20—H20···F3	0.95	2.54	3.181 (17)	125

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

1,3-Benzothiazole-2-thiol–1,2,3,5-tetrafluoro-4,6-diiodobenzene (1/1) (MBZTH_13F4DIB)

Crystal data

$C_6F_4I_2·C_7H_5NS_2$
M_r = 569.10
Triclinic, $P\overline{1}$
a = 7.2175 (4) Å
b = 8.2675 (5) Å
c = 14.4498 (9) Å
α = 97.936 (2)°
β = 91.297 (2)°
γ = 109.178 (2)°
V = 804.44 (8) Å^3
Z = 2
$F(000)$ = 528
D_x = 2.349 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9969 reflections
θ = 2.6–30.1°
μ = 4.20 mm^{-1}
T = 100 K
Plate, colourless
0.33 × 0.27 × 0.06 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec IμS
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.496, T_{max} = 0.746
27899 measured reflections

4701 independent reflections
4391 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 30.1°$, $\theta_{min} = 2.6°$
$h = -10 \rightarrow 10$
$k = -11 \rightarrow 11$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.018$
$wR(F^2) = 0.044$
$S = 1.09$
4701 reflections
203 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0115P)^2 + 0.801P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 1.08$ e Å^{-3}
$\Delta\rho_{min} = -1.11$ e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.21928 (2)	0.04578 (2)	0.73577 (2)	0.02046 (4)
I2	0.40359 (2)	0.24728 (2)	0.35536 (2)	0.02203 (4)
F1	0.17793 (18)	0.11993 (18)	0.52937 (9)	0.0275 (3)
F2	0.83758 (19)	0.35764 (19)	0.45929 (9)	0.0317 (3)
F3	0.95882 (18)	0.33437 (18)	0.63449 (9)	0.0304 (3)
F4	0.69486 (18)	0.19590 (15)	0.75449 (8)	0.0219 (2)
C8	0.4287 (3)	0.1563 (2)	0.64457 (13)	0.0174 (3)
C9	0.3711 (3)	0.1745 (3)	0.55526 (13)	0.0192 (4)
C10	0.5038 (3)	0.2421 (2)	0.49121 (13)	0.0184 (3)
C11	0.7028 (3)	0.2946 (3)	0.51885 (14)	0.0207 (4)
C12	0.7664 (3)	0.2813 (3)	0.60795 (14)	0.0209 (4)
C13	0.6289 (3)	0.2109 (2)	0.66928 (12)	0.0180 (3)
S1	0.82694 (7)	0.91230 (6)	0.86324 (3)	0.01549 (8)
S2	0.65916 (6)	0.53019 (5)	0.86630 (3)	0.01339 (8)
N1	0.8612 (2)	0.74012 (19)	1.00562 (10)	0.0127 (3)
HN1	0.938 (4)	0.835 (4)	1.0386 (19)	0.027 (7)*
C1	0.7938 (2)	0.7398 (2)	0.91829 (12)	0.0126 (3)
C2	0.7006 (2)	0.4453 (2)	0.96579 (12)	0.0127 (3)
C3	0.6389 (3)	0.2736 (2)	0.98130 (13)	0.0165 (3)
H3	0.563536	0.182216	0.934125	0.020*
C4	0.6913 (3)	0.2405 (2)	1.06823 (14)	0.0185 (3)
H4	0.650289	0.124547	1.080638	0.022*
C5	0.8032 (3)	0.3749 (2)	1.13778 (13)	0.0172 (3)
H5	0.836221	0.348582	1.196613	0.021*
C6	0.8667 (3)	0.5457 (2)	1.12210 (13)	0.0150 (3)
H6	0.943886	0.636838	1.168951	0.018*

C7	0.8134 (2)	0.5792 (2)	1.03532 (12)	0.0128 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.02600 (7)	0.02230 (6)	0.01536 (6)	0.00997 (5)	0.00446 (4)	0.00537 (4)
I2	0.03060 (7)	0.02527 (7)	0.01257 (6)	0.01186 (5)	−0.00081 (5)	0.00492 (4)
F1	0.0198 (6)	0.0426 (7)	0.0197 (6)	0.0086 (5)	−0.0015 (4)	0.0078 (5)
F2	0.0252 (6)	0.0391 (7)	0.0221 (6)	−0.0032 (5)	0.0029 (5)	0.0105 (5)
F3	0.0199 (6)	0.0372 (7)	0.0270 (7)	0.0003 (5)	−0.0064 (5)	0.0059 (5)
F4	0.0294 (6)	0.0222 (6)	0.0134 (5)	0.0085 (5)	−0.0059 (4)	0.0017 (4)
C8	0.0223 (9)	0.0171 (8)	0.0132 (8)	0.0072 (7)	0.0010 (6)	0.0024 (6)
C9	0.0202 (9)	0.0214 (9)	0.0149 (8)	0.0064 (7)	−0.0019 (6)	0.0009 (7)
C10	0.0242 (9)	0.0171 (8)	0.0126 (8)	0.0055 (7)	−0.0027 (7)	0.0023 (6)
C11	0.0232 (9)	0.0190 (9)	0.0163 (9)	0.0019 (7)	0.0018 (7)	0.0037 (7)
C12	0.0196 (9)	0.0196 (9)	0.0194 (9)	0.0020 (7)	−0.0037 (7)	0.0020 (7)
C13	0.0275 (9)	0.0147 (8)	0.0107 (8)	0.0066 (7)	−0.0029 (7)	−0.0005 (6)
S1	0.0184 (2)	0.01360 (18)	0.01265 (19)	0.00228 (15)	−0.00070 (15)	0.00408 (15)
S2	0.01404 (19)	0.01277 (18)	0.01164 (18)	0.00286 (14)	−0.00167 (14)	0.00058 (14)
N1	0.0128 (7)	0.0128 (6)	0.0110 (6)	0.0022 (5)	−0.0004 (5)	0.0018 (5)
C1	0.0124 (7)	0.0134 (7)	0.0117 (7)	0.0041 (6)	0.0017 (6)	0.0017 (6)
C2	0.0105 (7)	0.0143 (7)	0.0137 (7)	0.0044 (6)	0.0014 (6)	0.0029 (6)
C3	0.0145 (8)	0.0126 (7)	0.0209 (9)	0.0030 (6)	0.0001 (6)	0.0021 (6)
C4	0.0183 (8)	0.0150 (8)	0.0232 (9)	0.0052 (7)	0.0026 (7)	0.0073 (7)
C5	0.0158 (8)	0.0205 (8)	0.0184 (8)	0.0078 (7)	0.0020 (6)	0.0082 (7)
C6	0.0116 (7)	0.0184 (8)	0.0158 (8)	0.0055 (6)	0.0003 (6)	0.0039 (6)
C7	0.0115 (7)	0.0128 (7)	0.0142 (8)	0.0038 (6)	0.0018 (6)	0.0026 (6)

Geometric parameters (Å, º)

I1—C8	2.0910 (19)	S2—C2	1.7452 (18)
I2—C10	2.0875 (18)	N1—HN1	0.87 (3)
F1—C9	1.343 (2)	N1—C1	1.342 (2)
F2—C11	1.337 (2)	N1—C7	1.391 (2)
F3—C12	1.341 (2)	C2—C3	1.393 (2)
F4—C13	1.346 (2)	C2—C7	1.401 (2)
C8—C9	1.390 (3)	C3—H3	0.9500
C8—C13	1.387 (3)	C3—C4	1.392 (3)
C9—C10	1.385 (3)	C4—H4	0.9500
C10—C11	1.388 (3)	C4—C5	1.401 (3)
C11—C12	1.388 (3)	C5—H5	0.9500
C12—C13	1.383 (3)	C5—C6	1.387 (3)
S1—C1	1.6799 (18)	C6—H6	0.9500
S2—C1	1.7355 (18)	C6—C7	1.393 (2)
C9—C8—I1	120.65 (14)	S1—C1—S2	122.60 (10)
C13—C8—I1	122.00 (14)	N1—C1—S1	127.05 (13)
C13—C8—C9	117.34 (18)	N1—C1—S2	110.35 (13)

F1—C9—C8	118.30 (18)	C3—C2—S2	129.26 (14)
F1—C9—C10	118.70 (17)	C3—C2—C7	120.78 (16)
C10—C9—C8	122.97 (18)	C7—C2—S2	109.95 (13)
C9—C10—I2	120.15 (14)	C2—C3—H3	121.1
C9—C10—C11	117.73 (17)	C4—C3—C2	117.77 (17)
C11—C10—I2	121.99 (14)	C4—C3—H3	121.1
F2—C11—C10	120.33 (17)	C3—C4—H4	119.4
F2—C11—C12	118.58 (18)	C3—C4—C5	121.28 (17)
C12—C11—C10	121.09 (18)	C5—C4—H4	119.4
F3—C12—C11	120.72 (18)	C4—C5—H5	119.5
F3—C12—C13	120.01 (17)	C6—C5—C4	121.03 (17)
C13—C12—C11	119.27 (18)	C6—C5—H5	119.5
F4—C13—C8	120.41 (17)	C5—C6—H6	121.1
F4—C13—C12	118.00 (17)	C5—C6—C7	117.75 (16)
C12—C13—C8	121.59 (17)	C7—C6—H6	121.1
C1—S2—C2	91.89 (8)	N1—C7—C2	111.76 (15)
C1—N1—HN1	120.5 (18)	N1—C7—C6	126.87 (16)
C1—N1—C7	116.05 (15)	C6—C7—C2	121.37 (16)
C7—N1—HN1	123.3 (18)		

I1—C8—C9—F1	0.2 (2)	C13—C8—C9—F1	178.96 (17)
I1—C8—C9—C10	−178.06 (15)	C13—C8—C9—C10	0.7 (3)
I1—C8—C13—F4	−0.8 (2)	S2—C2—C3—C4	−179.54 (14)
I1—C8—C13—C12	178.95 (15)	S2—C2—C7—N1	−0.38 (18)
I2—C10—C11—F2	2.8 (3)	S2—C2—C7—C6	179.86 (13)
I2—C10—C11—C12	−176.43 (15)	C1—S2—C2—C3	−179.18 (17)
F1—C9—C10—I2	−2.9 (3)	C1—S2—C2—C7	0.60 (13)
F1—C9—C10—C11	−178.78 (18)	C1—N1—C7—C2	−0.2 (2)
F2—C11—C12—F3	1.6 (3)	C1—N1—C7—C6	179.60 (17)
F2—C11—C12—C13	−177.81 (18)	C2—S2—C1—S1	179.93 (12)
F3—C12—C13—F4	−0.9 (3)	C2—S2—C1—N1	−0.69 (13)
F3—C12—C13—C8	179.31 (17)	C2—C3—C4—C5	−0.4 (3)
C8—C9—C10—I2	175.43 (15)	C3—C2—C7—N1	179.42 (15)
C8—C9—C10—C11	−0.5 (3)	C3—C2—C7—C6	−0.3 (3)
C9—C8—C13—F4	−179.55 (16)	C3—C4—C5—C6	−0.4 (3)
C9—C8—C13—C12	0.2 (3)	C4—C5—C6—C7	0.7 (3)
C9—C10—C11—F2	178.66 (18)	C5—C6—C7—N1	179.90 (17)
C9—C10—C11—C12	−0.6 (3)	C5—C6—C7—C2	−0.4 (3)
C10—C11—C12—F3	−179.14 (18)	C7—N1—C1—S1	179.95 (13)
C10—C11—C12—C13	1.5 (3)	C7—N1—C1—S2	0.61 (19)
C11—C12—C13—F4	178.52 (17)	C7—C2—C3—C4	0.7 (3)
C11—C12—C13—C8	−1.3 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···S1^{i}	0.87 (3)	2.45 (3)	3.3120 (15)	175 (2)

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

1,3-Benzothiazole-2-thiol–1,2,3,5-tetrafluoro-4,6-diiodobenzene (1/2) (MBZTH_213F4DIB)

Crystal data

$4C_6F_4I_2{\cdot}2C_7H_5NS_2$
M_r = 1941.92
Monoclinic, $P2_1$
a = 4.5581 (3) Å
b = 34.358 (2) Å
c = 15.6075 (10) Å
β = 94.707 (2)°
V = 2436.0 (3) Å^3
Z = 2
$F(000)$ = 1768
D_x = 2.647 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9841 reflections
θ = 2.4–28.8°
μ = 5.36 mm^{-1}
T = 100 K
Prism, colourless
0.18 × 0.12 × 0.04 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec IμS
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.568, T_{max} = 0.746
56285 measured reflections
12660 independent reflections
11766 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 28.8°, θ_{min} = 2.2°
h = −6→6
k = −46→46
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.046
S = 1.09
12660 reflections
622 parameters
2 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0071P)^2 + 0.5877P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 1.01 e Å^{-3}
$\Delta\rho_{min}$ = −0.71 e Å^{-3}
Absolute structure: Refined as an inversion twin
Absolute structure parameter: 0.454 (15)

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. Refined as a 2-component inversion twin.

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

	x	y	z	U_{iso}*/U_{eq}
I1	1.31057 (9)	0.37856 (2)	0.44709 (3)	0.01694 (9)
I2	0.58291 (10)	0.34353 (2)	0.11336 (3)	0.02224 (10)
I3	0.13207 (9)	0.44552 (2)	0.04395 (3)	0.01659 (9)
I4	0.84342 (11)	0.47934 (2)	0.38106 (3)	0.02660 (11)
F1	1.0269 (9)	0.38363 (11)	0.2525 (2)	0.0233 (9)
F2	0.4263 (9)	0.27169 (12)	0.2331 (3)	0.0284 (10)

F3	0.6051 (10)	0.25383 (12)	0.3971 (3)	0.0324 (10)
F4	0.9918 (10)	0.29933 (12)	0.4890 (2)	0.0276 (10)
F5	0.3945 (8)	0.44111 (11)	0.2407 (2)	0.0205 (8)
F6	1.0552 (9)	0.54664 (12)	0.2573 (3)	0.0301 (10)
F7	0.9034 (9)	0.56331 (12)	0.0915 (3)	0.0331 (10)
F8	0.4927 (9)	0.52114 (12)	0.0003 (2)	0.0247 (9)
C15	1.0262 (13)	0.34210 (19)	0.3717 (4)	0.0147 (13)
C16	0.9275 (14)	0.35093 (18)	0.2876 (4)	0.0163 (13)
C17	0.7260 (13)	0.32806 (19)	0.2383 (4)	0.0150 (13)
C18	0.6246 (14)	0.2950 (2)	0.2766 (4)	0.0181 (14)
C19	0.7144 (15)	0.2853 (2)	0.3607 (4)	0.0197 (14)
C20	0.9139 (15)	0.3087 (2)	0.4070 (4)	0.0187 (14)
C21	0.4273 (13)	0.48043 (17)	0.1192 (4)	0.0118 (12)
C22	0.5141 (14)	0.47193 (19)	0.2048 (4)	0.0160 (13)
C23	0.7212 (14)	0.49397 (19)	0.2538 (4)	0.0170 (13)
C24	0.8475 (14)	0.5248 (2)	0.2137 (5)	0.0204 (15)
C25	0.7690 (15)	0.53442 (19)	0.1293 (5)	0.0207 (15)
C26	0.5582 (14)	0.51219 (19)	0.0829 (4)	0.0164 (13)
I5	0.60231 (10)	0.58298 (2)	0.42231 (3)	0.02666 (11)
I6	−0.04120 (12)	0.67426 (2)	0.67979 (3)	0.03213 (12)
F13	0.3626 (9)	0.61104 (13)	0.5966 (2)	0.0298 (9)
F14	−0.1966 (10)	0.72120 (12)	0.5061 (3)	0.0340 (11)
F15	−0.0233 (11)	0.71370 (13)	0.3475 (3)	0.0379 (11)
F16	0.3387 (10)	0.65460 (13)	0.3104 (3)	0.0340 (10)
C33	0.3592 (15)	0.63148 (19)	0.4533 (4)	0.0215 (14)
C34	0.2700 (15)	0.63678 (19)	0.5348 (4)	0.0212 (14)
C35	0.0859 (15)	0.6674 (2)	0.5562 (4)	0.0215 (15)
C36	−0.0098 (16)	0.6922 (2)	0.4907 (5)	0.0241 (15)
C37	0.0756 (16)	0.6885 (2)	0.4086 (5)	0.0267 (16)
C38	0.2587 (16)	0.6584 (2)	0.3901 (4)	0.0241 (15)
I7	0.27675 (10)	0.60812 (2)	−0.10563 (3)	0.02281 (10)
I8	1.08854 (10)	0.74677 (2)	−0.05335 (3)	0.02152 (10)
F9	0.6582 (9)	0.68287 (11)	−0.1413 (2)	0.0239 (9)
F10	1.0852 (9)	0.71219 (12)	0.1364 (2)	0.0286 (10)
F11	0.7847 (10)	0.65341 (14)	0.2015 (2)	0.0365 (11)
F12	0.4105 (9)	0.61029 (12)	0.0985 (3)	0.0293 (9)
C27	0.5318 (14)	0.64475 (18)	−0.0249 (4)	0.0164 (13)
C28	0.6884 (14)	0.67579 (19)	−0.0565 (4)	0.0166 (13)
C29	0.8730 (13)	0.69920 (18)	−0.0044 (4)	0.0165 (13)
C30	0.9054 (15)	0.6911 (2)	0.0830 (4)	0.0219 (15)
C31	0.7507 (16)	0.6609 (2)	0.1168 (4)	0.0233 (15)
C32	0.5630 (14)	0.63862 (19)	0.0628 (4)	0.0202 (14)
S1	0.6754 (4)	0.40568 (5)	0.88863 (11)	0.0189 (3)
S2	1.0703 (4)	0.33606 (5)	0.91405 (10)	0.0186 (3)
N1	0.9694 (12)	0.36855 (16)	0.7688 (3)	0.0152 (11)
HN1	0.905 (14)	0.3871 (19)	0.732 (4)	0.007 (16)*
C1	0.8985 (13)	0.37204 (18)	0.8506 (4)	0.0151 (13)
C2	1.1602 (14)	0.33784 (19)	0.7534 (4)	0.0162 (13)

C3	1.2632 (16)	0.3281 (2)	0.6749 (4)	0.0236 (15)
H3	1.206730	0.342708	0.624462	0.028*
C4	1.4504 (15)	0.2966 (2)	0.6723 (4)	0.0261 (16)
H4	1.525655	0.289582	0.619464	0.031*
C5	1.5310 (15)	0.2748 (2)	0.7462 (5)	0.0262 (16)
H5	1.657929	0.253028	0.742875	0.031*
C6	1.4270 (15)	0.28477 (19)	0.8243 (4)	0.0201 (14)
H6	1.483893	0.270321	0.874871	0.024*
C7	1.2378 (14)	0.31638 (19)	0.8270 (4)	0.0168 (13)
S3	0.7312 (4)	0.42496 (5)	0.60016 (10)	0.0190 (3)
S4	0.3357 (4)	0.49495 (5)	0.57647 (10)	0.0180 (3)
N2	0.4180 (12)	0.45945 (16)	0.7190 (3)	0.0164 (12)
HN2	0.497 (15)	0.449 (2)	0.764 (3)	0.03 (2)*
C8	0.4996 (14)	0.45745 (19)	0.6383 (4)	0.0162 (13)
C9	0.2219 (14)	0.48927 (19)	0.7357 (4)	0.0174 (13)
C10	0.1004 (14)	0.4970 (2)	0.8131 (4)	0.0190 (14)
H10	0.149370	0.481541	0.862699	0.023*
C11	−0.0915 (15)	0.5276 (2)	0.8154 (4)	0.0221 (15)
H11	−0.179266	0.533075	0.867172	0.027*
C12	−0.1615 (15)	0.5510 (2)	0.7427 (4)	0.0208 (14)
H12	−0.295108	0.572001	0.746348	0.025*
C13	−0.0391 (14)	0.5439 (2)	0.6659 (4)	0.0220 (15)
H13	−0.083511	0.560008	0.617145	0.026*
C14	0.1515 (13)	0.51230 (19)	0.6627 (4)	0.0158 (13)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.0177 (2)	0.0159 (2)	0.01700 (19)	0.00011 (16)	0.00007 (16)	−0.00234 (17)
I2	0.0263 (2)	0.0245 (2)	0.0153 (2)	0.00547 (19)	−0.00254 (18)	−0.00115 (18)
I3	0.0171 (2)	0.0170 (2)	0.01558 (19)	0.00146 (16)	0.00089 (16)	−0.00224 (17)
I4	0.0313 (3)	0.0303 (3)	0.0169 (2)	0.0123 (2)	−0.00624 (19)	−0.00536 (19)
F1	0.032 (2)	0.019 (2)	0.0194 (19)	−0.0084 (17)	0.0019 (17)	0.0046 (17)
F2	0.028 (2)	0.029 (2)	0.027 (2)	−0.0075 (18)	−0.0056 (18)	−0.0054 (19)
F3	0.041 (3)	0.023 (2)	0.033 (2)	−0.0147 (19)	−0.001 (2)	0.0100 (19)
F4	0.040 (3)	0.025 (2)	0.0168 (19)	−0.0053 (19)	−0.0029 (18)	0.0056 (17)
F5	0.029 (2)	0.016 (2)	0.0167 (18)	−0.0053 (17)	0.0061 (16)	0.0037 (16)
F6	0.019 (2)	0.029 (2)	0.042 (3)	−0.0079 (18)	−0.0024 (19)	−0.010 (2)
F7	0.032 (2)	0.024 (2)	0.044 (3)	−0.0084 (19)	0.011 (2)	0.010 (2)
F8	0.029 (2)	0.028 (2)	0.0170 (19)	−0.0002 (18)	0.0002 (17)	0.0100 (17)
C15	0.010 (3)	0.016 (3)	0.019 (3)	0.000 (2)	0.002 (2)	−0.001 (3)
C16	0.017 (3)	0.013 (3)	0.020 (3)	0.001 (2)	0.005 (3)	0.003 (3)
C17	0.013 (3)	0.021 (4)	0.011 (3)	0.002 (3)	0.000 (2)	−0.001 (3)
C18	0.016 (3)	0.019 (4)	0.018 (3)	−0.002 (3)	−0.001 (3)	−0.002 (3)
C19	0.021 (4)	0.017 (4)	0.021 (3)	−0.004 (3)	0.004 (3)	−0.001 (3)
C20	0.024 (4)	0.017 (4)	0.014 (3)	0.004 (3)	0.001 (3)	0.001 (3)
C21	0.017 (3)	0.009 (3)	0.010 (3)	0.001 (2)	0.003 (2)	−0.001 (2)
C22	0.018 (3)	0.015 (3)	0.016 (3)	0.001 (3)	0.007 (3)	0.001 (3)

C23	0.017 (3)	0.016 (3)	0.016 (3)	0.004 (3)	−0.003 (3)	−0.002 (3)
C24	0.012 (3)	0.021 (4)	0.028 (4)	0.000 (3)	0.000 (3)	−0.008 (3)
C25	0.018 (3)	0.009 (3)	0.035 (4)	−0.002 (3)	0.007 (3)	0.006 (3)
C26	0.014 (3)	0.017 (3)	0.018 (3)	−0.001 (3)	0.004 (3)	0.002 (3)
I5	0.0251 (2)	0.0252 (3)	0.0291 (2)	0.00486 (19)	−0.00180 (19)	−0.0083 (2)
I6	0.0376 (3)	0.0383 (3)	0.0218 (2)	0.0001 (2)	0.0099 (2)	−0.0023 (2)
F13	0.037 (2)	0.029 (2)	0.024 (2)	0.002 (2)	0.0010 (19)	0.0053 (19)
F14	0.034 (3)	0.031 (3)	0.038 (2)	0.014 (2)	0.012 (2)	0.000 (2)
F15	0.047 (3)	0.033 (3)	0.032 (2)	0.005 (2)	−0.002 (2)	0.019 (2)
F16	0.036 (3)	0.045 (3)	0.021 (2)	0.009 (2)	0.0073 (19)	0.0024 (19)
C33	0.022 (4)	0.016 (3)	0.027 (4)	0.001 (3)	0.003 (3)	−0.004 (3)
C34	0.024 (4)	0.019 (4)	0.021 (3)	−0.005 (3)	−0.001 (3)	0.003 (3)
C35	0.024 (4)	0.021 (4)	0.021 (3)	−0.002 (3)	0.011 (3)	−0.003 (3)
C36	0.021 (4)	0.020 (4)	0.031 (4)	−0.001 (3)	0.002 (3)	−0.002 (3)
C37	0.023 (4)	0.030 (4)	0.028 (4)	0.001 (3)	0.006 (3)	0.008 (3)
C38	0.027 (4)	0.030 (4)	0.016 (3)	−0.001 (3)	0.006 (3)	0.002 (3)
I7	0.0204 (2)	0.0188 (2)	0.0290 (2)	−0.00085 (18)	−0.00007 (19)	−0.00546 (19)
I8	0.0220 (2)	0.0161 (2)	0.0263 (2)	−0.00127 (17)	0.00103 (18)	0.00192 (18)
F9	0.029 (2)	0.025 (2)	0.0171 (19)	−0.0009 (17)	−0.0005 (17)	−0.0004 (16)
F10	0.028 (2)	0.036 (3)	0.021 (2)	−0.0123 (19)	0.0001 (18)	−0.0051 (18)
F11	0.039 (3)	0.052 (3)	0.018 (2)	−0.013 (2)	0.0041 (19)	0.004 (2)
F12	0.026 (2)	0.030 (2)	0.034 (2)	−0.0084 (19)	0.0099 (19)	0.006 (2)
C27	0.015 (3)	0.009 (3)	0.025 (3)	−0.001 (2)	−0.002 (3)	−0.005 (3)
C28	0.018 (3)	0.016 (3)	0.015 (3)	0.003 (3)	0.001 (3)	0.002 (3)
C29	0.010 (3)	0.012 (3)	0.027 (3)	−0.001 (2)	0.004 (3)	−0.003 (3)
C30	0.018 (3)	0.027 (4)	0.021 (3)	−0.002 (3)	0.001 (3)	−0.005 (3)
C31	0.025 (4)	0.030 (4)	0.015 (3)	0.002 (3)	0.002 (3)	0.000 (3)
C32	0.017 (3)	0.016 (3)	0.030 (4)	0.000 (3)	0.010 (3)	0.000 (3)
S1	0.0189 (8)	0.0203 (9)	0.0175 (8)	0.0005 (7)	0.0009 (7)	−0.0035 (7)
S2	0.0224 (8)	0.0197 (9)	0.0134 (7)	−0.0011 (7)	−0.0004 (6)	0.0024 (6)
N1	0.022 (3)	0.014 (3)	0.010 (2)	0.000 (2)	0.000 (2)	0.002 (2)
C1	0.013 (3)	0.016 (3)	0.016 (3)	−0.004 (2)	0.000 (2)	−0.001 (3)
C2	0.015 (3)	0.017 (3)	0.016 (3)	−0.004 (3)	−0.002 (3)	−0.003 (3)
C3	0.024 (4)	0.030 (4)	0.016 (3)	0.001 (3)	0.002 (3)	0.001 (3)
C4	0.019 (4)	0.035 (4)	0.023 (4)	0.003 (3)	−0.003 (3)	−0.008 (3)
C5	0.017 (4)	0.027 (4)	0.033 (4)	0.004 (3)	−0.004 (3)	−0.008 (3)
C6	0.021 (4)	0.019 (4)	0.020 (3)	0.000 (3)	−0.003 (3)	−0.002 (3)
C7	0.016 (3)	0.018 (3)	0.015 (3)	−0.002 (3)	−0.004 (3)	−0.004 (3)
S3	0.0190 (8)	0.0206 (9)	0.0172 (8)	−0.0007 (7)	0.0001 (7)	−0.0018 (7)
S4	0.0191 (8)	0.0217 (9)	0.0129 (7)	−0.0017 (7)	0.0002 (6)	0.0016 (6)
N2	0.013 (3)	0.020 (3)	0.015 (3)	−0.001 (2)	−0.002 (2)	0.003 (2)
C8	0.017 (3)	0.018 (3)	0.013 (3)	−0.007 (3)	−0.001 (3)	−0.001 (2)
C9	0.017 (3)	0.019 (3)	0.015 (3)	−0.005 (3)	−0.004 (3)	−0.002 (3)
C10	0.021 (3)	0.022 (4)	0.014 (3)	−0.006 (3)	0.003 (3)	0.001 (3)
C11	0.026 (4)	0.025 (4)	0.016 (3)	−0.006 (3)	0.007 (3)	−0.008 (3)
C12	0.018 (3)	0.019 (4)	0.025 (4)	0.000 (3)	0.003 (3)	−0.006 (3)
C13	0.017 (3)	0.022 (4)	0.026 (4)	−0.003 (3)	−0.004 (3)	0.003 (3)
C14	0.011 (3)	0.020 (3)	0.015 (3)	−0.004 (3)	−0.002 (3)	−0.003 (3)

Geometric parameters (Å, º)

I1—C15	2.094 (6)	F11—C31	1.344 (7)
I2—C17	2.075 (6)	F12—C32	1.343 (7)
I3—C21	2.090 (6)	C27—C28	1.396 (9)
I4—C23	2.080 (6)	C27—C32	1.381 (9)
F1—C16	1.345 (7)	C28—C29	1.379 (9)
F2—C18	1.349 (8)	C29—C30	1.387 (9)
F3—C19	1.336 (7)	C30—C31	1.383 (9)
F4—C20	1.338 (7)	C31—C32	1.382 (10)
F5—C22	1.335 (7)	S1—C1	1.679 (6)
F6—C24	1.348 (8)	S2—C1	1.730 (7)
F7—C25	1.330 (7)	S2—C7	1.748 (7)
F8—C26	1.336 (7)	N1—HN1	0.89 (6)
C15—C16	1.386 (9)	N1—C1	1.347 (7)
C15—C20	1.389 (9)	N1—C2	1.401 (8)
C16—C17	1.391 (9)	C2—C3	1.389 (9)
C17—C18	1.381 (9)	C2—C7	1.385 (9)
C18—C19	1.383 (9)	C3—H3	0.9500
C19—C20	1.373 (10)	C3—C4	1.382 (10)
C21—C22	1.393 (8)	C4—H4	0.9500
C21—C26	1.387 (8)	C4—C5	1.398 (10)
C22—C23	1.389 (9)	C5—H5	0.9500
C23—C24	1.380 (10)	C5—C6	1.387 (9)
C24—C25	1.377 (10)	C6—H6	0.9500
C25—C26	1.384 (9)	C6—C7	1.390 (9)
I5—C33	2.080 (6)	S3—C8	1.679 (7)
I6—C35	2.073 (6)	S4—C8	1.741 (7)
F13—C34	1.351 (8)	S4—C14	1.748 (6)
F14—C36	1.346 (8)	N2—HN2	0.85 (3)
F15—C37	1.339 (8)	N2—C8	1.343 (8)
F16—C38	1.331 (7)	N2—C9	1.398 (8)
C33—C34	1.380 (9)	C9—C10	1.396 (9)
C33—C38	1.400 (10)	C9—C14	1.403 (9)
C34—C35	1.402 (9)	C10—H10	0.9500
C35—C36	1.373 (10)	C10—C11	1.369 (10)
C36—C37	1.375 (10)	C11—H11	0.9500
C37—C38	1.375 (10)	C11—C12	1.405 (9)
I7—C27	2.069 (6)	C12—H12	0.9500
I8—C29	2.085 (6)	C12—C13	1.384 (9)
F9—C28	1.342 (7)	C13—H13	0.9500
F10—C30	1.334 (8)	C13—C14	1.394 (9)
C16—C15—I1	122.6 (5)	C28—C29—C30	118.2 (6)
C16—C15—C20	117.1 (6)	C30—C29—I8	120.1 (5)
C20—C15—I1	120.2 (5)	F10—C30—C29	121.1 (6)
F1—C16—C15	118.3 (6)	F10—C30—C31	118.4 (6)
F1—C16—C17	118.4 (6)	C31—C30—C29	120.6 (6)

C15—C16—C17	123.2 (6)	F11—C31—C30	119.9 (6)
C16—C17—I2	121.1 (5)	F11—C31—C32	120.5 (6)
C18—C17—I2	121.8 (5)	C32—C31—C30	119.6 (6)
C18—C17—C16	117.1 (6)	F12—C32—C27	120.5 (6)
F2—C18—C17	120.3 (6)	F12—C32—C31	117.7 (6)
F2—C18—C19	118.0 (6)	C27—C32—C31	121.8 (6)
C17—C18—C19	121.7 (6)	C1—S2—C7	92.2 (3)
F3—C19—C18	120.4 (6)	C1—N1—HN1	117 (4)
F3—C19—C20	120.2 (6)	C1—N1—C2	115.5 (5)
C20—C19—C18	119.3 (6)	C2—N1—HN1	127 (4)
F4—C20—C15	120.0 (6)	S1—C1—S2	123.3 (4)
F4—C20—C19	118.3 (6)	N1—C1—S1	126.5 (5)
C19—C20—C15	121.6 (6)	N1—C1—S2	110.2 (5)
C22—C21—I3	122.5 (5)	C3—C2—N1	126.3 (6)
C26—C21—I3	120.1 (4)	C7—C2—N1	112.2 (6)
C26—C21—C22	117.3 (6)	C7—C2—C3	121.5 (6)
F5—C22—C21	118.4 (6)	C2—C3—H3	121.1
F5—C22—C23	118.9 (6)	C4—C3—C2	117.9 (6)
C23—C22—C21	122.7 (6)	C4—C3—H3	121.1
C22—C23—I4	120.7 (5)	C3—C4—H4	119.4
C24—C23—I4	122.0 (5)	C3—C4—C5	121.1 (7)
C24—C23—C22	117.3 (6)	C5—C4—H4	119.4
F6—C24—C23	120.0 (6)	C4—C5—H5	119.8
F6—C24—C25	117.8 (6)	C6—C5—C4	120.5 (7)
C25—C24—C23	122.2 (6)	C6—C5—H5	119.8
F7—C25—C24	120.7 (6)	C5—C6—H6	120.8
F7—C25—C26	120.3 (6)	C5—C6—C7	118.5 (6)
C24—C25—C26	118.9 (6)	C7—C6—H6	120.8
F8—C26—C21	120.4 (6)	C2—C7—S2	109.9 (5)
F8—C26—C25	117.9 (6)	C2—C7—C6	120.5 (6)
C25—C26—C21	121.6 (6)	C6—C7—S2	129.6 (5)
C34—C33—I5	121.5 (5)	C8—S4—C14	92.1 (3)
C34—C33—C38	117.3 (6)	C8—N2—HN2	129 (5)
C38—C33—I5	121.0 (5)	C8—N2—C9	116.3 (6)
F13—C34—C33	118.3 (6)	C9—N2—HN2	113 (5)
F13—C34—C35	118.6 (6)	S3—C8—S4	123.3 (4)
C33—C34—C35	123.1 (6)	N2—C8—S3	126.7 (5)
C34—C35—I6	121.7 (5)	N2—C8—S4	110.0 (5)
C36—C35—I6	121.7 (5)	N2—C9—C14	111.7 (6)
C36—C35—C34	116.6 (6)	C10—C9—N2	127.3 (6)
F14—C36—C35	119.6 (6)	C10—C9—C14	121.0 (6)
F14—C36—C37	117.8 (6)	C9—C10—H10	121.0
C35—C36—C37	122.6 (7)	C11—C10—C9	117.9 (6)
F15—C37—C36	120.0 (6)	C11—C10—H10	121.0
F15—C37—C38	120.8 (6)	C10—C11—H11	119.3
C38—C37—C36	119.2 (7)	C10—C11—C12	121.4 (6)
F16—C38—C33	119.7 (6)	C12—C11—H11	119.3
F16—C38—C37	119.1 (6)	C11—C12—H12	119.4

C37—C38—C33	121.2 (6)	C13—C12—C11	121.2 (6)
C28—C27—I7	121.9 (5)	C13—C12—H12	119.4
C32—C27—I7	121.2 (5)	C12—C13—H13	121.1
C32—C27—C28	116.9 (6)	C12—C13—C14	117.7 (6)
F9—C28—C27	118.2 (6)	C14—C13—H13	121.1
F9—C28—C29	118.9 (6)	C9—C14—S4	109.9 (5)
C29—C28—C27	122.9 (6)	C13—C14—S4	129.3 (5)
C28—C29—I8	121.6 (5)	C13—C14—C9	120.7 (6)

I1—C15—C16—F1	2.2 (8)	C35—C36—C37—C38	1.5 (11)
I1—C15—C16—C17	−176.3 (5)	C36—C37—C38—F16	179.3 (6)
I1—C15—C20—F4	−1.3 (8)	C36—C37—C38—C33	0.0 (11)
I1—C15—C20—C19	176.4 (5)	C38—C33—C34—F13	179.5 (6)
I2—C17—C18—F2	−0.2 (9)	C38—C33—C34—C35	0.1 (10)
I2—C17—C18—C19	−178.3 (5)	I7—C27—C28—F9	3.5 (8)
I3—C21—C22—F5	−2.7 (8)	I7—C27—C28—C29	−176.2 (5)
I3—C21—C22—C23	176.7 (5)	I7—C27—C32—F12	−4.9 (9)
I3—C21—C26—F8	1.3 (8)	I7—C27—C32—C31	174.8 (5)
I3—C21—C26—C25	−175.7 (5)	I8—C29—C30—F10	−3.5 (9)
I4—C23—C24—F6	−0.5 (9)	I8—C29—C30—C31	176.4 (5)
I4—C23—C24—C25	179.5 (5)	F9—C28—C29—I8	3.1 (8)
F1—C16—C17—I2	0.4 (8)	F9—C28—C29—C30	−179.0 (6)
F1—C16—C17—C18	−179.0 (6)	F10—C30—C31—F11	−0.2 (10)
F2—C18—C19—F3	−0.4 (10)	F10—C30—C31—C32	−179.9 (6)
F2—C18—C19—C20	−179.4 (6)	F11—C31—C32—F12	2.2 (10)
F3—C19—C20—F4	−0.8 (10)	F11—C31—C32—C27	−177.6 (6)
F3—C19—C20—C15	−178.5 (6)	C27—C28—C29—I8	−177.3 (5)
F5—C22—C23—I4	−0.1 (8)	C27—C28—C29—C30	0.6 (10)
F5—C22—C23—C24	177.8 (6)	C28—C27—C32—F12	177.4 (6)
F6—C24—C25—F7	2.8 (10)	C28—C27—C32—C31	−2.9 (10)
F6—C24—C25—C26	179.4 (6)	C28—C29—C30—F10	178.6 (6)
F7—C25—C26—F8	−1.0 (10)	C28—C29—C30—C31	−1.5 (10)
F7—C25—C26—C21	176.0 (6)	C29—C30—C31—F11	179.9 (6)
C15—C16—C17—I2	179.0 (5)	C29—C30—C31—C32	0.2 (10)
C15—C16—C17—C18	−0.4 (10)	C30—C31—C32—F12	−178.1 (6)
C16—C15—C20—F4	−177.5 (6)	C30—C31—C32—C27	2.1 (10)
C16—C15—C20—C19	0.2 (10)	C32—C27—C28—F9	−178.8 (6)
C16—C17—C18—F2	179.2 (6)	C32—C27—C28—C29	1.5 (10)
C16—C17—C18—C19	1.2 (10)	N1—C2—C3—C4	−179.8 (6)
C17—C18—C19—F3	177.7 (6)	N1—C2—C7—S2	−0.7 (7)
C17—C18—C19—C20	−1.3 (11)	N1—C2—C7—C6	−179.7 (6)
C18—C19—C20—F4	178.3 (6)	C1—S2—C7—C2	0.5 (5)
C18—C19—C20—C15	0.6 (10)	C1—S2—C7—C6	179.4 (7)
C20—C15—C16—F1	178.3 (5)	C1—N1—C2—C3	179.5 (6)
C20—C15—C16—C17	−0.2 (10)	C1—N1—C2—C7	0.6 (8)
C21—C22—C23—I4	−179.5 (5)	C2—N1—C1—S1	−179.8 (5)
C21—C22—C23—C24	−1.5 (10)	C2—N1—C1—S2	−0.2 (7)
C22—C21—C26—F8	177.6 (6)	C2—C3—C4—C5	0.8 (11)

C22—C21—C26—C25	0.7 (9)	C3—C2—C7—S2	−179.7 (5)
C22—C23—C24—F6	−178.3 (6)	C3—C2—C7—C6	1.3 (10)
C22—C23—C24—C25	1.6 (10)	C3—C4—C5—C6	−0.8 (11)
C23—C24—C25—F7	−177.2 (6)	C4—C5—C6—C7	1.1 (10)
C23—C24—C25—C26	−0.6 (10)	C5—C6—C7—S2	179.9 (5)
C24—C25—C26—F8	−177.7 (6)	C5—C6—C7—C2	−1.3 (10)
C24—C25—C26—C21	−0.6 (10)	C7—S2—C1—S1	179.5 (4)
C26—C21—C22—F5	−178.9 (5)	C7—S2—C1—N1	−0.2 (5)
C26—C21—C22—C23	0.4 (9)	C7—C2—C3—C4	−1.0 (10)
I5—C33—C34—F13	4.8 (9)	N2—C9—C10—C11	−179.2 (6)
I5—C33—C34—C35	−174.6 (5)	N2—C9—C14—S4	0.3 (7)
I5—C33—C38—F16	−5.4 (9)	N2—C9—C14—C13	−179.4 (6)
I5—C33—C38—C37	174.0 (6)	C8—S4—C14—C9	0.4 (5)
I6—C35—C36—F14	−1.7 (10)	C8—S4—C14—C13	−180.0 (6)
I6—C35—C36—C37	178.9 (6)	C8—N2—C9—C10	178.6 (6)
F13—C34—C35—I6	0.9 (9)	C8—N2—C9—C14	−1.1 (8)
F13—C34—C35—C36	−178.2 (6)	C9—N2—C8—S3	179.9 (5)
F14—C36—C37—F15	1.1 (10)	C9—N2—C8—S4	1.4 (7)
F14—C36—C37—C38	−177.9 (7)	C9—C10—C11—C12	−1.0 (10)
F15—C37—C38—F16	0.4 (11)	C10—C9—C14—S4	−179.5 (5)
F15—C37—C38—C33	−179.0 (7)	C10—C9—C14—C13	0.8 (10)
C33—C34—C35—I6	−179.8 (5)	C10—C11—C12—C13	0.2 (11)
C33—C34—C35—C36	1.2 (10)	C11—C12—C13—C14	1.2 (10)
C34—C33—C38—F16	179.9 (6)	C12—C13—C14—S4	178.7 (5)
C34—C33—C38—C37	−0.8 (11)	C12—C13—C14—C9	−1.7 (10)
C34—C35—C36—F14	177.3 (6)	C14—S4—C8—S3	−179.6 (4)
C34—C35—C36—C37	−2.0 (11)	C14—S4—C8—N2	−1.0 (5)
C35—C36—C37—F15	−179.5 (7)	C14—C9—C10—C11	0.5 (10)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···S3	0.89 (6)	2.51 (6)	3.376 (6)	165 (5)
C3—H3···I1	0.95	3.10	3.976 (7)	154
N2—H*N*2···S1	0.85 (3)	2.52 (3)	3.360 (6)	169 (7)
C10—H10···I3^{i}	0.95	3.09	4.006 (6)	161

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

1,3-Benzothiazole-2-thiol–1,2,4,5-tetrafluoro-3,6-diiodobenzene (2/1) (2MBZTH_14F4DIB)

Crystal data

$C_6F_4I_2·2C_7H_5NS_2$
M_r = 736.34
Monoclinic, $P2_1/n$
a = 5.5057 (2) Å
b = 15.6087 (7) Å
c = 13.5194 (6) Å
β = 94.259 (2)°
V = 1158.61 (8) Å^3
Z = 2
F(000) = 700
D_x = 2.111 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9937 reflections
θ = 2.6–30.1°

μ = 3.12 mm^{-1}
T = 100 K

Needle, colourless
0.17 × 0.09 × 0.04 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec IμS
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.559, T_{max} = 0.746
22270 measured reflections

3402 independent reflections
2811 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 30.1°, θ_{min} = 2.6°
h = −7→7
k = −22→21
l = −18→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.057
S = 1.15
3402 reflections
149 parameters
0 restraints
Primary atom site location: dual

Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0092P)^2 + 1.689P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.90 e Å^{-3}
$\Delta\rho_{min}$ = −0.78 e Å^{-3}

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.

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

	x	y	z	U_{iso}*/U_{eq}
I1	0.09620 (3)	0.50667 (2)	0.18841 (2)	0.01843 (6)
F1	0.4987 (3)	0.36936 (10)	0.13226 (14)	0.0285 (4)
F2	0.8063 (3)	0.36478 (10)	−0.00971 (13)	0.0267 (4)
C8	0.3371 (5)	0.50280 (17)	0.0761 (2)	0.0179 (5)
C9	0.4956 (5)	0.43488 (17)	0.0673 (2)	0.0210 (6)
C10	0.6546 (5)	0.43202 (17)	−0.0070 (2)	0.0190 (5)
S1	−0.29400 (12)	0.50758 (4)	0.36239 (5)	0.01927 (14)
S2	0.07419 (13)	0.64355 (4)	0.42496 (5)	0.02067 (15)
N1	−0.2698 (4)	0.60239 (14)	0.52996 (18)	0.0175 (5)
HN1	−0.379 (6)	0.577 (2)	0.548 (3)	0.024 (9)*
C1	−0.1812 (5)	0.58112 (16)	0.4433 (2)	0.0166 (5)
C2	−0.1450 (5)	0.66593 (16)	0.5855 (2)	0.0173 (5)
C3	−0.2004 (5)	0.69814 (17)	0.6767 (2)	0.0225 (6)
H3	−0.337581	0.678027	0.708502	0.027*
C4	−0.0491 (6)	0.76050 (19)	0.7197 (2)	0.0271 (7)
H4	−0.083090	0.783531	0.782261	0.032*
C5	0.1516 (6)	0.79028 (19)	0.6737 (2)	0.0269 (7)
H5	0.253410	0.832708	0.705534	0.032*
C6	0.2060 (5)	0.75900 (17)	0.5816 (2)	0.0237 (6)

H6	0.342177	0.779762	0.549629	0.028*
C7	0.0542 (5)	0.69629 (16)	0.5379 (2)	0.0178 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01632 (9)	0.02275 (9)	0.01671 (10)	0.00025 (7)	0.00446 (6)	−0.00296 (6)
F1	0.0349 (10)	0.0250 (8)	0.0273 (10)	0.0077 (7)	0.0135 (8)	0.0069 (7)
F2	0.0284 (9)	0.0247 (8)	0.0283 (10)	0.0099 (7)	0.0107 (8)	0.0003 (7)
C8	0.0152 (12)	0.0226 (13)	0.0162 (14)	−0.0007 (10)	0.0035 (10)	−0.0063 (10)
C9	0.0216 (14)	0.0217 (13)	0.0200 (15)	−0.0003 (11)	0.0031 (12)	−0.0003 (10)
C10	0.0169 (12)	0.0196 (12)	0.0207 (15)	0.0022 (10)	0.0019 (11)	−0.0047 (10)
S1	0.0194 (3)	0.0228 (3)	0.0161 (3)	−0.0054 (3)	0.0047 (3)	−0.0013 (2)
S2	0.0195 (3)	0.0236 (3)	0.0198 (4)	−0.0062 (3)	0.0071 (3)	−0.0005 (3)
N1	0.0170 (11)	0.0165 (10)	0.0196 (13)	−0.0033 (9)	0.0057 (9)	0.0011 (9)
C1	0.0154 (12)	0.0176 (12)	0.0170 (14)	−0.0002 (10)	0.0030 (10)	0.0036 (9)
C2	0.0189 (13)	0.0148 (11)	0.0184 (14)	−0.0022 (10)	0.0016 (11)	0.0020 (9)
C3	0.0227 (14)	0.0226 (13)	0.0230 (16)	0.0016 (11)	0.0061 (12)	0.0009 (11)
C4	0.0322 (16)	0.0254 (14)	0.0238 (17)	0.0003 (12)	0.0036 (13)	−0.0066 (12)
C5	0.0273 (15)	0.0221 (14)	0.0307 (18)	−0.0041 (12)	−0.0022 (13)	−0.0029 (12)
C6	0.0232 (14)	0.0194 (13)	0.0286 (17)	−0.0051 (11)	0.0023 (12)	0.0013 (11)
C7	0.0173 (12)	0.0170 (12)	0.0193 (15)	−0.0007 (10)	0.0027 (11)	0.0026 (10)

Geometric parameters (Å, º)

I1—C8	2.090 (3)	N1—C2	1.394 (4)
F1—C9	1.348 (3)	C2—C3	1.386 (4)
F2—C10	1.344 (3)	C2—C7	1.395 (4)
C8—C9	1.384 (4)	C3—H3	0.9500
C8—C10^{i}	1.385 (4)	C3—C4	1.381 (4)
C9—C10	1.381 (4)	C4—H4	0.9500
S1—C1	1.673 (3)	C4—C5	1.388 (4)
S2—C1	1.743 (3)	C5—H5	0.9500
S2—C7	1.746 (3)	C5—C6	1.390 (4)
N1—HN1	0.78 (3)	C6—H6	0.9500
N1—C1	1.344 (3)	C6—C7	1.390 (4)
C9—C8—I1	121.6 (2)	C3—C2—N1	127.2 (2)
C9—C8—C10^{i}	116.8 (2)	C3—C2—C7	121.3 (3)
C10^{i}—C8—I1	121.59 (19)	C2—C3—H3	121.2
F1—C9—C8	120.2 (2)	C4—C3—C2	117.7 (3)
F1—C9—C10	118.1 (2)	C4—C3—H3	121.2
C10—C9—C8	121.7 (3)	C3—C4—H4	119.3
F2—C10—C8^{i}	120.2 (2)	C3—C4—C5	121.5 (3)
F2—C10—C9	118.3 (2)	C5—C4—H4	119.3
C9—C10—C8^{i}	121.4 (2)	C4—C5—H5	119.5
C1—S2—C7	92.03 (13)	C4—C5—C6	121.0 (3)
C1—N1—HN1	119 (3)	C6—C5—H5	119.5

C1—N1—C2	116.7 (2)	C5—C6—H6	121.1
C2—N1—HN1	124 (3)	C7—C6—C5	117.7 (3)
S1—C1—S2	123.72 (16)	C7—C6—H6	121.1
N1—C1—S1	126.7 (2)	C2—C7—S2	110.2 (2)
N1—C1—S2	109.5 (2)	C6—C7—S2	128.9 (2)
N1—C2—C7	111.5 (2)	C6—C7—C2	120.8 (3)
I1—C8—C9—F1	−0.5 (4)	C1—N1—C2—C7	0.3 (3)
I1—C8—C9—C10	179.8 (2)	C2—N1—C1—S1	−180.0 (2)
F1—C9—C10—F2	−0.9 (4)	C2—N1—C1—S2	−0.7 (3)
F1—C9—C10—C8^{i}	−179.6 (3)	C2—C3—C4—C5	0.1 (5)
C8—C9—C10—F2	178.7 (3)	C3—C2—C7—S2	−179.8 (2)
C8—C9—C10—C8^{i}	0.0 (5)	C3—C2—C7—C6	1.1 (4)
C10^{i}—C8—C9—F1	179.6 (3)	C3—C4—C5—C6	0.8 (5)
C10^{i}—C8—C9—C10	0.0 (5)	C4—C5—C6—C7	−0.7 (5)
N1—C2—C3—C4	179.0 (3)	C5—C6—C7—S2	−179.2 (2)
N1—C2—C7—S2	0.2 (3)	C5—C6—C7—C2	−0.2 (4)
N1—C2—C7—C6	−178.9 (3)	C7—S2—C1—S1	180.00 (19)
C1—S2—C7—C2	−0.5 (2)	C7—S2—C1—N1	0.7 (2)
C1—S2—C7—C6	178.5 (3)	C7—C2—C3—C4	−1.0 (4)
C1—N1—C2—C3	−179.7 (3)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···S1^{ii}	0.78 (3)	2.60 (3)	3.369 (2)	170 (3)
C3—H3···F1^{iii}	0.95	2.50	3.333 (3)	146
C6—H6···F2^{iv}	0.95	2.44	3.357 (3)	162

Symmetry codes: (ii) −*x*−1, −*y*+1, −*z*+1; (iii) −*x*, −*y*+1, −*z*+1; (iv) −*x*+3/2, *y*+1/2, −*z*+1/2.

1,3-Benzothiazole-2-thiol–1,3,5-trifluoro-2,4,6-triiodobenzene (1/1) (MBZTH_135F3I3B)

Crystal data

$C_6F_3I_3·C_7H_5NS_2$
M_r = 677.00
Monoclinic, $P2_1/c$
a = 15.2665 (6) Å
b = 4.7380 (2) Å
c = 23.2215 (10) Å
β = 93.139 (2)°
V = 1677.15 (12) Å^3
Z = 4
$F(000)$ = 1232
D_x = 2.681 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9894 reflections
θ = 3.1–28.4°
μ = 5.86 mm^{-1}
T = 100 K
Plate, colourless
0.16 × 0.08 × 0.05 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec IμS
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.610, T_{max} = 0.746
35222 measured reflections
4212 independent reflections

3611 reflections with $I > 2\sigma(I)$
$R_{int} = 0.057$
$\theta_{max} = 28.4°$, $\theta_{min} = 2.2°$
$h = -19 \rightarrow 20$
$k = -6 \rightarrow 6$
$l = -30 \rightarrow 31$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.024$
$wR(F^2) = 0.052$
$S = 1.18$
4212 reflections
203 parameters
1 restraint
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + 4.0997P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 0.67$ e Å^{-3}
$\Delta\rho_{min} = -0.73$ e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.70161 (2)	0.58105 (5)	0.55847 (2)	0.01897 (6)
I2	0.68104 (2)	−0.18871 (6)	0.76567 (2)	0.02456 (7)
I3	0.37648 (2)	−0.11384 (6)	0.58903 (2)	0.02243 (6)
F1	0.75133 (13)	0.2505 (5)	0.67513 (9)	0.0224 (5)
F2	0.49679 (14)	−0.2816 (5)	0.70076 (9)	0.0247 (5)
F3	0.51145 (13)	0.3138 (5)	0.54048 (9)	0.0224 (5)
C8	0.6317 (2)	0.2972 (7)	0.60769 (15)	0.0161 (7)
C9	0.6683 (2)	0.1805 (8)	0.65793 (15)	0.0168 (7)
C10	0.6242 (2)	−0.0129 (8)	0.69039 (15)	0.0170 (7)
C11	0.5404 (2)	−0.0910 (8)	0.67047 (15)	0.0195 (7)
C12	0.5008 (2)	0.0172 (8)	0.62016 (15)	0.0170 (7)
C13	0.5477 (2)	0.2102 (8)	0.58980 (15)	0.0177 (7)
S1	0.85079 (6)	1.0132 (2)	0.49475 (4)	0.02217 (19)
S2	0.81182 (6)	0.6044 (2)	0.39819 (4)	0.02095 (19)
N1	0.9677 (2)	0.7071 (7)	0.43672 (13)	0.0205 (6)
HN1	1.011 (2)	0.777 (10)	0.4571 (18)	0.040 (14)*
C1	0.8842 (2)	0.7835 (8)	0.44595 (15)	0.0185 (7)
C2	0.9777 (2)	0.5076 (8)	0.39362 (16)	0.0203 (7)
C3	1.0556 (3)	0.3935 (9)	0.37636 (18)	0.0278 (9)
H3	1.110354	0.453291	0.393589	0.033*
C4	1.0518 (3)	0.1913 (9)	0.33364 (18)	0.0303 (9)
H4	1.104619	0.107792	0.322010	0.036*
C5	0.9720 (3)	0.1072 (9)	0.30721 (18)	0.0304 (9)
H5	0.971216	−0.031349	0.277614	0.036*
C6	0.8934 (3)	0.2228 (8)	0.32348 (17)	0.0260 (8)
H6	0.838874	0.165478	0.305463	0.031*
C7	0.8970 (2)	0.4256 (8)	0.36705 (15)	0.0194 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01882 (12)	0.01952 (12)	0.01885 (12)	−0.00162 (9)	0.00346 (9)	−0.00136 (9)
I2	0.02741 (13)	0.02835 (14)	0.01735 (12)	0.00846 (10)	−0.00403 (9)	0.00139 (10)
I3	0.01542 (11)	0.03132 (14)	0.02042 (12)	−0.00464 (9)	−0.00022 (9)	−0.00501 (10)
F1	0.0151 (10)	0.0285 (12)	0.0230 (11)	−0.0008 (9)	−0.0039 (8)	−0.0038 (9)
F2	0.0261 (11)	0.0259 (12)	0.0221 (11)	−0.0066 (9)	0.0014 (9)	0.0078 (9)
F3	0.0198 (10)	0.0286 (12)	0.0184 (10)	0.0021 (9)	−0.0027 (8)	0.0066 (9)
C8	0.0174 (16)	0.0146 (17)	0.0163 (16)	−0.0009 (13)	0.0025 (13)	−0.0019 (13)
C9	0.0137 (16)	0.0191 (17)	0.0175 (17)	0.0018 (13)	−0.0010 (13)	−0.0058 (14)
C10	0.0180 (17)	0.0184 (17)	0.0142 (16)	0.0044 (13)	−0.0036 (13)	−0.0014 (14)
C11	0.0206 (18)	0.0202 (18)	0.0180 (17)	−0.0001 (14)	0.0032 (14)	−0.0004 (14)
C12	0.0130 (16)	0.0198 (18)	0.0180 (17)	−0.0001 (13)	0.0000 (13)	−0.0020 (14)
C13	0.0159 (16)	0.0208 (18)	0.0163 (16)	0.0037 (14)	0.0007 (13)	−0.0005 (14)
S1	0.0217 (5)	0.0233 (5)	0.0217 (5)	−0.0019 (4)	0.0019 (4)	−0.0025 (4)
S2	0.0158 (4)	0.0237 (5)	0.0229 (5)	−0.0027 (3)	−0.0021 (3)	−0.0020 (4)
N1	0.0183 (15)	0.0251 (17)	0.0178 (15)	−0.0035 (13)	−0.0019 (12)	−0.0011 (13)
C1	0.0178 (17)	0.0183 (18)	0.0191 (17)	−0.0026 (14)	−0.0004 (14)	0.0025 (14)
C2	0.0218 (18)	0.0196 (18)	0.0194 (18)	0.0014 (14)	−0.0019 (14)	0.0022 (15)
C3	0.0201 (19)	0.033 (2)	0.030 (2)	0.0003 (16)	−0.0023 (16)	0.0032 (18)
C4	0.033 (2)	0.031 (2)	0.028 (2)	0.0097 (18)	0.0072 (17)	0.0002 (18)
C5	0.043 (3)	0.022 (2)	0.026 (2)	0.0013 (18)	0.0067 (18)	−0.0007 (17)
C6	0.033 (2)	0.022 (2)	0.0223 (19)	−0.0059 (16)	−0.0037 (16)	0.0010 (16)
C7	0.0198 (18)	0.0199 (18)	0.0183 (17)	−0.0008 (14)	0.0004 (14)	0.0026 (14)

Geometric parameters (Å, º)

I1—C8	2.095 (3)	S2—C7	1.742 (4)
I2—C10	2.082 (3)	N1—HN1	0.857 (19)
I3—C12	2.088 (3)	N1—C1	1.353 (5)
F1—C9	1.349 (4)	N1—C2	1.391 (5)
F2—C11	1.343 (4)	C2—C3	1.386 (5)
F3—C13	1.338 (4)	C2—C7	1.402 (5)
C8—C9	1.381 (5)	C3—H3	0.9500
C8—C13	1.389 (5)	C3—C4	1.378 (6)
C9—C10	1.384 (5)	C4—H4	0.9500
C10—C11	1.388 (5)	C4—C5	1.393 (6)
C11—C12	1.384 (5)	C5—H5	0.9500
C12—C13	1.379 (5)	C5—C6	1.390 (6)
S1—C1	1.671 (4)	C6—H6	0.9500
S2—C1	1.743 (4)	C6—C7	1.394 (5)
C9—C8—I1	121.6 (3)	S1—C1—S2	122.8 (2)
C9—C8—C13	117.3 (3)	N1—C1—S1	127.4 (3)
C13—C8—I1	121.1 (3)	N1—C1—S2	109.8 (3)
F1—C9—C8	118.8 (3)	N1—C2—C7	112.1 (3)
F1—C9—C10	118.6 (3)	C3—C2—N1	127.1 (4)

C8—C9—C10	122.6 (3)	C3—C2—C7	120.8 (4)
C9—C10—I2	122.0 (3)	C2—C3—H3	120.8
C9—C10—C11	117.5 (3)	C4—C3—C2	118.5 (4)
C11—C10—I2	120.5 (3)	C4—C3—H3	120.8
F2—C11—C10	118.6 (3)	C3—C4—H4	119.4
F2—C11—C12	119.0 (3)	C3—C4—C5	121.1 (4)
C12—C11—C10	122.3 (3)	C5—C4—H4	119.4
C11—C12—I3	121.9 (3)	C4—C5—H5	119.5
C13—C12—I3	120.5 (3)	C6—C5—C4	121.0 (4)
C13—C12—C11	117.6 (3)	C6—C5—H5	119.5
F3—C13—C8	118.7 (3)	C5—C6—H6	121.0
F3—C13—C12	118.6 (3)	C5—C6—C7	117.9 (4)
C12—C13—C8	122.7 (3)	C7—C6—H6	121.0
C7—S2—C1	92.24 (18)	C2—C7—S2	109.9 (3)
C1—N1—HN1	121 (3)	C6—C7—S2	129.5 (3)
C1—N1—C2	115.9 (3)	C6—C7—C2	120.6 (3)
C2—N1—HN1	123 (3)		

I1—C8—C9—F1	−0.5 (4)	C13—C8—C9—F1	177.0 (3)
I1—C8—C9—C10	−178.3 (3)	C13—C8—C9—C10	−0.8 (5)
I1—C8—C13—F3	−0.7 (4)	N1—C2—C3—C4	178.2 (4)
I1—C8—C13—C12	178.0 (3)	N1—C2—C7—S2	−0.2 (4)
I2—C10—C11—F2	0.1 (5)	N1—C2—C7—C6	−178.7 (3)
I2—C10—C11—C12	−178.9 (3)	C1—S2—C7—C2	−0.2 (3)
I3—C12—C13—F3	0.8 (5)	C1—S2—C7—C6	178.1 (4)
I3—C12—C13—C8	−177.9 (3)	C1—N1—C2—C3	−179.4 (4)
F1—C9—C10—I2	1.7 (4)	C1—N1—C2—C7	0.8 (5)
F1—C9—C10—C11	−177.2 (3)	C2—N1—C1—S1	179.2 (3)
F2—C11—C12—I3	−1.4 (5)	C2—N1—C1—S2	−0.9 (4)
F2—C11—C12—C13	−179.3 (3)	C2—C3—C4—C5	1.5 (6)
C8—C9—C10—I2	179.5 (3)	C3—C2—C7—S2	179.9 (3)
C8—C9—C10—C11	0.6 (5)	C3—C2—C7—C6	1.4 (6)
C9—C8—C13—F3	−178.2 (3)	C3—C4—C5—C6	−0.6 (6)
C9—C8—C13—C12	0.4 (5)	C4—C5—C6—C7	0.0 (6)
C9—C10—C11—F2	179.0 (3)	C5—C6—C7—S2	−178.6 (3)
C9—C10—C11—C12	0.0 (5)	C5—C6—C7—C2	−0.4 (6)
C10—C11—C12—I3	177.6 (3)	C7—S2—C1—S1	−179.5 (2)
C10—C11—C12—C13	−0.4 (5)	C7—S2—C1—N1	0.6 (3)
C11—C12—C13—F3	178.8 (3)	C7—C2—C3—C4	−1.9 (6)
C11—C12—C13—C8	0.1 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···S1^{i}	0.86 (2)	2.54 (2)	3.389 (3)	172 (4)
C3—H3···I1^{ii}	0.95	3.03	3.928 (4)	159

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

1,3-Benzothiazole-2-thiol–1,1,2,2-tetraiodoethene (1/1) (MBZTH_TIE)

Crystal data

$C_2I_4 \cdot C_7H_5NS_2$
$M_r = 698.86$
Triclinic, $P\overline{1}$
$a = 7.4085$ (6) Å
$b = 10.8180$ (9) Å
$c = 11.1989$ (10) Å
$\alpha = 66.616$ (3)°
$\beta = 70.765$ (3)°
$\gamma = 70.792$ (3)°
$V = 757.20$ (11) Å^3
$Z = 2$
$F(000) = 620$
$D_x = 3.065$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9908 reflections
$\theta = 2.4$–$27.6°$
$\mu = 8.48$ mm^{-1}
$T = 100$ K
Block, yellow
0.08 × 0.07 × 0.07 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec IμS
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
$T_{min} = 0.589$, $T_{max} = 0.746$
22463 measured reflections
3484 independent reflections
3037 reflections with $I > 2\sigma(I)$
$R_{int} = 0.052$
$\theta_{max} = 27.6°$, $\theta_{min} = 2.1°$
$h = -9 \rightarrow 9$
$k = -14 \rightarrow 14$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.072$
$S = 1.13$
3484 reflections
159 parameters
7 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0264P)^2 + 3.2353P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 1.43$ e Å^{-3}
$\Delta\rho_{min} = -1.76$ e Å^{-3}

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.

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

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
I1	0.18703 (5)	0.90012 (3)	0.68231 (3)	0.02172 (9)	
I2	0.32280 (5)	0.95731 (4)	0.33480 (3)	0.02290 (9)	
C8	0.0936 (8)	0.9743 (5)	0.5033 (6)	0.0239 (11)	
I3	0.72172 (6)	0.21253 (4)	0.95745 (4)	0.03285 (11)	
I4	0.76779 (5)	−0.15110 (4)	1.05340 (4)	0.02545 (10)	
C9A	0.9080 (15)	0.0083 (10)	1.0028 (9)	0.016 (3)	0.529 (19)
C9B	0.9990 (16)	−0.0669 (12)	1.0232 (11)	0.016 (3)	0.471 (19)
S1	0.33205 (18)	0.46883 (15)	0.92558 (14)	0.0257 (3)	
S2	0.34982 (18)	0.53599 (14)	0.63493 (13)	0.0224 (3)	

N1	0.0271 (6)	0.5607 (5)	0.8065 (4)	0.0207 (9)
HN1	−0.057 (8)	0.555 (7)	0.881 (4)	0.036 (19)*
C1	0.2213 (7)	0.5214 (5)	0.7989 (5)	0.0193 (10)
C2	0.1323 (7)	0.6027 (5)	0.5783 (5)	0.0189 (10)
C3	0.1076 (8)	0.6481 (6)	0.4478 (6)	0.0245 (11)
H3	0.217056	0.642904	0.374510	0.029*
C4	−0.0808 (9)	0.7004 (6)	0.4295 (6)	0.0270 (12)
H4	−0.101730	0.733475	0.341722	0.032*
C5	−0.2416 (8)	0.7059 (6)	0.5370 (6)	0.0272 (12)
H5	−0.369991	0.742518	0.520859	0.033*
C6	−0.2192 (8)	0.6593 (5)	0.6671 (6)	0.0233 (11)
H6	−0.329217	0.662174	0.740411	0.028*
C7	−0.0280 (7)	0.6081 (5)	0.6852 (5)	0.0187 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01984 (17)	0.02418 (18)	0.02146 (18)	−0.00095 (13)	−0.00713 (13)	−0.00908 (13)
I2	0.01628 (16)	0.02862 (19)	0.02166 (18)	−0.00312 (13)	−0.00118 (13)	−0.01016 (14)
C8	0.024 (3)	0.020 (2)	0.025 (3)	0.002 (2)	−0.006 (2)	−0.009 (2)
I3	0.0351 (2)	0.0308 (2)	0.0316 (2)	0.01363 (16)	−0.01664 (17)	−0.01885 (16)
I4	0.02582 (18)	0.02565 (18)	0.02593 (19)	−0.01160 (14)	−0.00886 (14)	−0.00245 (14)
C9A	0.020 (5)	0.005 (4)	0.016 (4)	0.003 (4)	−0.004 (3)	−0.001 (3)
C9B	0.009 (5)	0.012 (6)	0.019 (5)	0.003 (4)	−0.004 (4)	−0.003 (4)
S1	0.0144 (6)	0.0329 (7)	0.0213 (6)	0.0021 (5)	−0.0034 (5)	−0.0067 (6)
S2	0.0158 (6)	0.0261 (6)	0.0215 (6)	−0.0002 (5)	−0.0008 (5)	−0.0105 (5)
N1	0.017 (2)	0.021 (2)	0.019 (2)	−0.0026 (17)	−0.0031 (17)	−0.0042 (18)
C1	0.016 (2)	0.015 (2)	0.024 (3)	−0.0034 (18)	−0.004 (2)	−0.005 (2)
C2	0.017 (2)	0.018 (2)	0.022 (3)	−0.0040 (19)	−0.0020 (19)	−0.008 (2)
C3	0.026 (3)	0.026 (3)	0.022 (3)	−0.005 (2)	−0.002 (2)	−0.012 (2)
C4	0.031 (3)	0.024 (3)	0.025 (3)	−0.009 (2)	−0.005 (2)	−0.005 (2)
C5	0.025 (3)	0.021 (3)	0.034 (3)	0.000 (2)	−0.012 (2)	−0.006 (2)
C6	0.019 (2)	0.020 (2)	0.029 (3)	−0.002 (2)	−0.004 (2)	−0.008 (2)
C7	0.020 (2)	0.015 (2)	0.018 (2)	−0.0022 (18)	−0.002 (2)	−0.0051 (19)

Geometric parameters (Å, º)

I1—C8	2.101 (6)	N1—C1	1.343 (6)
I2—C8	2.106 (6)	N1—C7	1.396 (7)
C8—C8^{i}	1.329 (11)	C2—C3	1.400 (8)
I3—C9A	2.146 (10)	C2—C7	1.386 (7)
I3—C9B^{ii}	2.166 (11)	C3—H3	0.9500
I4—C9A	2.095 (10)	C3—C4	1.373 (8)
I4—C9B	2.069 (11)	C4—H4	0.9500
C9A—C9A^{ii}	1.30 (2)	C4—C5	1.392 (8)
C9B—C9B^{ii}	1.33 (2)	C5—H5	0.9500
S1—C1	1.682 (5)	C5—C6	1.388 (8)
S2—C1	1.738 (5)	C6—H6	0.9500

S2—C2	1.750 (5)	C6—C7	1.392 (7)
N1—HN1	0.85 (2)		
I1—C8—I2	114.1 (2)	C7—C2—S2	109.9 (4)
C8^{i}—C8—I1	123.2 (6)	C7—C2—C3	121.0 (5)
C8^{i}—C8—I2	122.8 (6)	C2—C3—H3	121.2
C9A—I3—C9B^{ii}	26.4 (4)	C4—C3—C2	117.6 (5)
I4—C9A—I3	114.6 (5)	C4—C3—H3	121.2
C9A^{ii}—C9A—I3	120.0 (10)	C3—C4—H4	119.4
C9A^{ii}—C9A—I4	125.3 (10)	C3—C4—C5	121.3 (6)
I4—C9B—I3^{ii}	115.8 (5)	C5—C4—H4	119.4
C9B^{ii}—C9B—I4	127.1 (11)	C4—C5—H5	119.2
C1—S2—C2	91.8 (2)	C6—C5—C4	121.7 (5)
C1—N1—HN1	122 (5)	C6—C5—H5	119.2
C1—N1—C7	115.7 (4)	C5—C6—H6	121.5
C7—N1—HN1	122 (5)	C5—C6—C7	116.9 (5)
S1—C1—S2	123.1 (3)	C7—C6—H6	121.5
N1—C1—S1	126.6 (4)	C2—C7—N1	112.4 (4)
N1—C1—S2	110.2 (4)	C2—C7—C6	121.5 (5)
C3—C2—S2	129.1 (4)	C6—C7—N1	126.1 (5)
S2—C2—C3—C4	−178.0 (4)	C3—C2—C7—N1	−178.9 (5)
S2—C2—C7—N1	0.4 (5)	C3—C2—C7—C6	−0.3 (8)
S2—C2—C7—C6	179.0 (4)	C3—C4—C5—C6	0.2 (9)
C1—S2—C2—C3	177.8 (5)	C4—C5—C6—C7	0.7 (8)
C1—S2—C2—C7	−1.4 (4)	C5—C6—C7—N1	177.7 (5)
C1—N1—C7—C2	1.3 (6)	C5—C6—C7—C2	−0.7 (8)
C1—N1—C7—C6	−177.3 (5)	C7—N1—C1—S1	176.2 (4)
C2—S2—C1—S1	−176.4 (3)	C7—N1—C1—S2	−2.3 (6)
C2—S2—C1—N1	2.1 (4)	C7—C2—C3—C4	1.2 (8)
C2—C3—C4—C5	−1.1 (8)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···S1^{iii}	0.85 (2)	2.43 (2)	3.275 (5)	170 (6)

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

supporting information

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Halogen, chalcogen, and hydrogen bonding in organoiodine cocrystals of heterocyclic thiones: imidazolidine-2-thione, 2-mercaptobenzimidazole, 2-mercapto-5-methylbenzimidazole, 2-mercaptobenzoxazole, and 2-mercaptobenzothiazole

Spencer Watts, Andrew J. Peloquin, Madhushi Bandara, Colin D. McMillen and William T. Pennington

Computing details

For all structures, data collection: *APEX3* (Bruker, 2017); cell refinement: *SAINT* (Bruker, 2017); data reduction: *SAINT* (Bruker, 2017); program(s) used to solve structure: SHELXT2018 (Sheldrick, 2015*a*); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015*b*). Molecular graphics: *Mercury* (Macrae *et al.*, 2020) for 2IT_13F4DIB, 4MBZIM_313F4DIB, MBZIM_14F4DIB, MBZIM_TIE, MMBZIM_12F4DIB, 2MMBZIM_14F4DIB_2H2O, MMBZIM_135F3I3B, MBZOX_12F4DIB, MBZOX_13F4DIB, 2MBZOX_14F4DIB, MBZOX_135F3I3B, 3MBZTH_412F4DIB, MBZTH_13F4DIB, MBZTH_213F4DIB, 2MBZTH_14F4DIB, MBZTH_135F3I3B, MBZTH_TIE; OLEX2 (Dolomanov *et al.*, 2009) for IT_135F3I3B. For all structures, software used to prepare material for publication: OLEX2 (Dolomanov *et al.*, 2009).

1,2,3,5-Tetrafluoro-4,6-diiodobenzene–imidazolidine-2-thione (1/2) (2IT_13F4DIB)

Crystal data

$C_6F_4I_2·2C_3H_6N_2S$
M_r = 606.18
Orthorhombic, *Pbcn*
a = 15.6704 (7) Å
b = 8.9924 (4) Å
c = 26.0573 (10) Å
V = 3671.9 (3) Å^3
Z = 8
$F(000)$ = 2288
D_x = 2.193 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9343 reflections
θ = 2.6–30.1°
μ = 3.69 mm^{-1}
T = 100 K
Block, colourless
0.18 × 0.17 × 0.13 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec IμS
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.639, T_{max} = 0.746
112821 measured reflections
5376 independent reflections
5198 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 30.1°, θ_{min} = 2.0°
h = −22→22
k = −12→12
l = −36→31

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.015$
$wR(F^2) = 0.032$
$S = 1.25$
5376 reflections
234 parameters
0 restraints
Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0054P)^2 + 3.3158P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 0.42$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ e Å^{-3}
Extinction correction: SHELXL2018 (Sheldrick, 2015*b*), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00082 (4)

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.71842 (2)	0.27502 (2)	0.20785 (2)	0.01326 (3)
I2	0.98485 (2)	0.54110 (2)	0.35028 (2)	0.01761 (3)
F1	0.89456 (6)	0.34626 (11)	0.26335 (4)	0.01975 (19)
F2	0.81145 (7)	0.69420 (11)	0.38910 (4)	0.0230 (2)
F3	0.64754 (6)	0.66108 (12)	0.36116 (4)	0.0232 (2)
F4	0.60595 (6)	0.48196 (12)	0.28175 (4)	0.0215 (2)
C7	0.74984 (10)	0.40891 (16)	0.27097 (5)	0.0139 (3)
C8	0.83358 (10)	0.42536 (17)	0.28725 (6)	0.0145 (3)
C9	0.85758 (10)	0.51990 (17)	0.32680 (6)	0.0157 (3)
C10	0.79313 (10)	0.59875 (17)	0.35087 (6)	0.0165 (3)
C11	0.70856 (10)	0.58350 (18)	0.33669 (6)	0.0172 (3)
C12	0.68786 (10)	0.49038 (18)	0.29640 (6)	0.0155 (3)
S1	0.68567 (2)	0.95036 (4)	0.61354 (2)	0.01476 (7)
N1	0.69251 (9)	0.72075 (15)	0.54616 (5)	0.0166 (3)
HN1	0.7189 (14)	0.672 (3)	0.5672 (9)	0.027 (6)*
N2	0.64832 (10)	0.92951 (15)	0.51306 (5)	0.0182 (3)
HN2	0.6289 (14)	1.015 (2)	0.5136 (8)	0.022 (5)*
C1	0.67475 (9)	0.86294 (17)	0.55568 (6)	0.0134 (3)
C2	0.68382 (11)	0.68448 (18)	0.49167 (6)	0.0186 (3)
H2A	0.644157	0.600134	0.486460	0.022*
H2B	0.739772	0.659716	0.476228	0.022*
C3	0.64743 (11)	0.82909 (18)	0.46895 (6)	0.0199 (3)
H3A	0.683895	0.867131	0.440842	0.024*
H3B	0.588726	0.814231	0.455882	0.024*
S2	0.42217 (3)	0.71986 (5)	0.49680 (2)	0.02184 (9)
N3	0.47631 (10)	0.51791 (16)	0.42741 (5)	0.0199 (3)
HN3	0.4952 (13)	0.467 (2)	0.4491 (9)	0.020 (5)*
N4	0.40214 (9)	0.69778 (16)	0.39417 (5)	0.0173 (3)

HN4	0.3816 (15)	0.783 (3)	0.3921 (9)	0.028 (6)*
C4	0.43369 (10)	0.64323 (17)	0.43758 (6)	0.0150 (3)
C5	0.46475 (10)	0.47080 (17)	0.37446 (6)	0.0166 (3)
H5A	0.423029	0.388469	0.371861	0.020*
H5B	0.519445	0.439328	0.358855	0.020*
C6	0.43059 (11)	0.61337 (18)	0.34929 (6)	0.0180 (3)
H6A	0.476022	0.666661	0.330344	0.022*
H6B	0.382641	0.591836	0.325695	0.022*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01584 (5)	0.01297 (5)	0.01098 (4)	−0.00009 (3)	−0.00092 (3)	0.00036 (3)
I2	0.01801 (5)	0.01630 (5)	0.01853 (5)	−0.00213 (4)	−0.00276 (4)	−0.00185 (4)
F1	0.0169 (4)	0.0213 (5)	0.0210 (5)	0.0041 (4)	0.0008 (4)	−0.0073 (4)
F2	0.0276 (5)	0.0234 (5)	0.0182 (5)	−0.0016 (4)	0.0000 (4)	−0.0098 (4)
F3	0.0216 (5)	0.0265 (5)	0.0215 (5)	0.0042 (4)	0.0058 (4)	−0.0079 (4)
F4	0.0143 (4)	0.0284 (5)	0.0217 (5)	0.0006 (4)	0.0006 (4)	−0.0042 (4)
C7	0.0190 (7)	0.0121 (6)	0.0105 (6)	−0.0010 (5)	0.0006 (5)	0.0002 (5)
C8	0.0170 (7)	0.0124 (6)	0.0141 (6)	0.0019 (5)	0.0012 (5)	−0.0001 (5)
C9	0.0175 (7)	0.0140 (7)	0.0155 (7)	−0.0009 (5)	−0.0013 (5)	0.0000 (5)
C10	0.0222 (8)	0.0144 (7)	0.0128 (6)	−0.0015 (6)	0.0005 (6)	−0.0015 (5)
C11	0.0205 (7)	0.0159 (7)	0.0152 (7)	0.0022 (6)	0.0043 (6)	−0.0010 (6)
C12	0.0150 (7)	0.0167 (7)	0.0146 (6)	−0.0010 (6)	0.0007 (5)	0.0014 (5)
S1	0.01883 (17)	0.01408 (16)	0.01138 (15)	0.00309 (13)	−0.00079 (13)	0.00015 (13)
N1	0.0220 (7)	0.0127 (6)	0.0150 (6)	0.0032 (5)	−0.0018 (5)	0.0014 (5)
N2	0.0277 (7)	0.0133 (6)	0.0136 (6)	0.0055 (5)	−0.0030 (5)	−0.0008 (5)
C1	0.0119 (6)	0.0140 (6)	0.0142 (6)	0.0004 (5)	0.0011 (5)	0.0008 (5)
C2	0.0259 (8)	0.0148 (7)	0.0152 (7)	0.0014 (6)	0.0001 (6)	−0.0028 (6)
C3	0.0276 (8)	0.0180 (7)	0.0141 (7)	0.0030 (6)	−0.0023 (6)	−0.0026 (6)
S2	0.0339 (2)	0.01651 (18)	0.01508 (17)	0.01055 (16)	−0.00313 (16)	−0.00093 (14)
N3	0.0280 (7)	0.0164 (6)	0.0151 (6)	0.0094 (6)	−0.0051 (5)	0.0000 (5)
N4	0.0212 (7)	0.0146 (6)	0.0161 (6)	0.0054 (5)	−0.0028 (5)	0.0010 (5)
C4	0.0143 (7)	0.0127 (6)	0.0179 (7)	0.0004 (5)	−0.0011 (5)	0.0015 (5)
C5	0.0197 (7)	0.0139 (7)	0.0161 (7)	0.0018 (6)	0.0003 (6)	−0.0003 (5)
C6	0.0221 (8)	0.0167 (7)	0.0153 (7)	0.0043 (6)	−0.0022 (6)	0.0002 (6)

Geometric parameters (Å, º)

I1—C7	2.0969 (14)	N2—C3	1.462 (2)
I2—C9	2.0947 (16)	C2—H2A	0.9900
F1—C8	1.3442 (17)	C2—H2B	0.9900
F2—C10	1.3459 (17)	C2—C3	1.538 (2)
F3—C11	1.3445 (18)	C3—H3A	0.9900
F4—C12	1.3412 (18)	C3—H3B	0.9900
C7—C8	1.387 (2)	S2—C4	1.6995 (16)
C7—C12	1.385 (2)	N3—HN3	0.79 (2)
C8—C9	1.388 (2)	N3—C4	1.337 (2)

C9—C10	1.384 (2)	N3—C5	1.455 (2)
C10—C11	1.383 (2)	N4—HN4	0.83 (2)
C11—C12	1.382 (2)	N4—C4	1.328 (2)
S1—C1	1.7088 (15)	N4—C6	1.464 (2)
N1—HN1	0.81 (2)	C5—H5A	0.9900
N1—C1	1.332 (2)	C5—H5B	0.9900
N1—C2	1.463 (2)	C5—C6	1.536 (2)
N2—HN2	0.83 (2)	C6—H6A	0.9900
N2—C1	1.3280 (19)	C6—H6B	0.9900

C8—C7—I1	121.56 (11)	H2A—C2—H2B	109.1
C12—C7—I1	120.94 (11)	C3—C2—H2A	111.2
C12—C7—C8	117.43 (14)	C3—C2—H2B	111.2
F1—C8—C7	118.31 (13)	N2—C3—C2	102.49 (12)
F1—C8—C9	118.39 (14)	N2—C3—H3A	111.3
C7—C8—C9	123.29 (14)	N2—C3—H3B	111.3
C8—C9—I2	122.05 (11)	C2—C3—H3A	111.3
C10—C9—I2	121.04 (11)	C2—C3—H3B	111.3
C10—C9—C8	116.90 (14)	H3A—C3—H3B	109.2
F2—C10—C9	120.43 (14)	C4—N3—HN3	122.5 (16)
F2—C10—C11	117.74 (14)	C4—N3—C5	111.80 (13)
C11—C10—C9	121.83 (14)	C5—N3—HN3	124.0 (16)
F3—C11—C10	120.23 (14)	C4—N4—HN4	122.7 (16)
F3—C11—C12	120.52 (15)	C4—N4—C6	112.06 (13)
C12—C11—C10	119.23 (14)	C6—N4—HN4	122.8 (16)
F4—C12—C7	120.34 (14)	N3—C4—S2	125.10 (12)
F4—C12—C11	118.37 (14)	N4—C4—S2	125.73 (12)
C11—C12—C7	121.29 (15)	N4—C4—N3	109.17 (14)
C1—N1—HN1	119.7 (16)	N3—C5—H5A	111.4
C1—N1—C2	112.04 (13)	N3—C5—H5B	111.4
C2—N1—HN1	125.6 (16)	N3—C5—C6	101.85 (12)
C1—N2—HN2	121.3 (15)	H5A—C5—H5B	109.3
C1—N2—C3	112.46 (13)	C6—C5—H5A	111.4
C3—N2—HN2	125.8 (15)	C6—C5—H5B	111.4
N1—C1—S1	125.81 (12)	N4—C6—C5	101.41 (12)
N2—C1—S1	124.18 (12)	N4—C6—H6A	111.5
N2—C1—N1	110.01 (14)	N4—C6—H6B	111.5
N1—C2—H2A	111.2	C5—C6—H6A	111.5
N1—C2—H2B	111.2	C5—C6—H6B	111.5
N1—C2—C3	102.68 (12)	H6A—C6—H6B	109.3

I1—C7—C8—F1	−3.75 (19)	C9—C10—C11—C12	−1.9 (2)
I1—C7—C8—C9	175.92 (12)	C10—C11—C12—F4	−177.15 (14)
I1—C7—C12—F4	1.7 (2)	C10—C11—C12—C7	1.9 (2)
I1—C7—C12—C11	−177.34 (12)	C12—C7—C8—F1	179.43 (13)
I2—C9—C10—F2	1.9 (2)	C12—C7—C8—C9	−0.9 (2)
I2—C9—C10—C11	−178.45 (12)	N1—C2—C3—N2	4.94 (17)
F1—C8—C9—I2	−0.4 (2)	C1—N1—C2—C3	−5.82 (18)

F1—C8—C9—C10	−179.48 (14)	C1—N2—C3—C2	−2.96 (19)
F2—C10—C11—F3	−0.8 (2)	C2—N1—C1—S1	−174.62 (12)
F2—C10—C11—C12	177.76 (14)	C2—N1—C1—N2	4.27 (19)
F3—C11—C12—F4	1.4 (2)	C3—N2—C1—S1	178.31 (12)
F3—C11—C12—C7	−179.58 (14)	C3—N2—C1—N1	−0.6 (2)
C7—C8—C9—I2	179.89 (11)	N3—C5—C6—N4	−18.18 (16)
C7—C8—C9—C10	0.9 (2)	C4—N3—C5—C6	16.94 (18)
C8—C7—C12—F4	178.51 (14)	C4—N4—C6—C5	15.47 (18)
C8—C7—C12—C11	−0.5 (2)	C5—N3—C4—S2	172.13 (12)
C8—C9—C10—F2	−179.09 (14)	C5—N3—C4—N4	−7.96 (19)
C8—C9—C10—C11	0.6 (2)	C6—N4—C4—S2	174.32 (12)
C9—C10—C11—F3	179.53 (14)	C6—N4—C4—N3	−5.59 (19)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···S1^{i}	0.81 (2)	2.77 (2)	3.5551 (14)	163 (2)
N2—H*N*2···S2^{ii}	0.83 (2)	2.53 (2)	3.3507 (14)	172 (2)
C2—H2*B*···F2	0.99	2.55	3.3392 (19)	136
C3—H3*B*···S2	0.99	2.94	3.7351 (19)	138
N3—H*N*3···S2^{iii}	0.79 (2)	2.54 (2)	3.3171 (15)	167 (2)
N4—H*N*4···I2^{iv}	0.83 (2)	3.31 (2)	3.7383 (14)	114.9 (18)
N4—H*N*4···S1^{ii}	0.83 (2)	2.63 (2)	3.4562 (14)	179 (2)
C5—H5*A*···I1^{v}	0.99	3.20	3.9922 (16)	138
C5—H5*B*···F4	0.99	2.45	3.2774 (19)	140
C6—H6*B*···I1^{vi}	0.99	3.18	3.9223 (16)	133

Symmetry codes: (i) −*x*+3/2, *y*−1/2, *z*; (ii) −*x*+1, −*y*+2, −*z*+1; (iii) −*x*+1, −*y*+1, −*z*+1; (iv) −*x*+3/2, *y*+1/2, *z*; (v) −*x*+1, *y*, −*z*+1/2; (vi) *x*−1/2, *y*+1/2, −*z*+1/2.

Imidazolidine-2-thione–1,3,5-trifluoro-2,4,6-triiodobenzene (1/1) (IT_135F3I3B)

Crystal data

$C_6F_3I_3·C_3H_6N_2S$
M_r = 611.92
Orthorhombic, *Pbca*
a = 18.0407 (14) Å
b = 7.2816 (6) Å
c = 22.1250 (19) Å
V = 2906.5 (4) Å^3
Z = 8
F(000) = 2208
D_x = 2.797 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 9914 reflections
θ = 2.9–28.3°
μ = 6.61 mm^{-1}
T = 100 K
Tabular, colourless
0.22 × 0.08 × 0.04 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec I*μ*S
φ and *ω* scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.563, T_{max} = 0.746
49179 measured reflections
3615 independent reflections
3220 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 28.3°, θ_{min} = 2.2°
h = −24→24
k = −9→9
l = −28→29

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.019$
$wR(F^2) = 0.040$
$S = 1.11$
3615 reflections
172 parameters
2 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0114P)^2 + 5.9439P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.57$ e Å^{-3}
$\Delta\rho_{min} = -0.77$ e Å^{-3}
Extinction correction: SHELXL2018 (Sheldrick, 2015*b*), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.000108 (15)

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.53750 (2)	0.23369 (3)	0.54191 (2)	0.01895 (5)
I2	0.82382 (2)	0.16514 (2)	0.68496 (2)	0.01507 (5)
I3	0.83267 (2)	0.32805 (2)	0.41594 (2)	0.01451 (5)
F1	0.65074 (9)	0.1654 (2)	0.64879 (8)	0.0189 (4)
F2	0.88045 (8)	0.2474 (2)	0.55242 (8)	0.0197 (4)
F3	0.65981 (9)	0.3180 (2)	0.44277 (8)	0.0179 (3)
C4	0.65271 (14)	0.2418 (4)	0.54544 (13)	0.0139 (5)
C5	0.69034 (15)	0.2057 (4)	0.59879 (13)	0.0146 (5)
C6	0.76726 (14)	0.2079 (4)	0.60287 (13)	0.0135 (5)
C7	0.80537 (14)	0.2449 (4)	0.54993 (13)	0.0140 (5)
C8	0.77196 (14)	0.2814 (4)	0.49545 (13)	0.0133 (5)
C9	0.69470 (14)	0.2803 (4)	0.49494 (13)	0.0137 (5)
S1	0.57097 (4)	0.61400 (10)	0.79736 (3)	0.01671 (14)
N1	0.52694 (14)	0.2877 (4)	0.84174 (13)	0.0228 (6)
HN1	0.4953 (19)	0.345 (6)	0.8617 (18)	0.057 (14)*
N2	0.62179 (16)	0.2684 (4)	0.78288 (13)	0.0257 (6)
HN2	0.6527 (16)	0.308 (5)	0.7585 (14)	0.029 (10)*
C1	0.57324 (15)	0.3832 (4)	0.80740 (12)	0.0161 (6)
C2	0.54227 (16)	0.0908 (4)	0.84203 (14)	0.0222 (6)
H2A	0.498578	0.019283	0.828618	0.027*
H2B	0.557562	0.048198	0.882651	0.027*
C3	0.60613 (19)	0.0758 (4)	0.79654 (16)	0.0277 (7)
H3A	0.649751	0.014419	0.814660	0.033*
H3B	0.590783	0.007958	0.759844	0.033*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01058 (8)	0.02130 (10)	0.02496 (11)	0.00013 (7)	0.00038 (7)	−0.00336 (8)
I2	0.01700 (9)	0.01397 (9)	0.01424 (10)	−0.00039 (6)	−0.00190 (7)	0.00115 (7)
I3	0.01480 (8)	0.01468 (9)	0.01405 (9)	0.00001 (6)	0.00204 (7)	0.00044 (7)
F1	0.0176 (8)	0.0235 (9)	0.0157 (9)	−0.0029 (7)	0.0045 (7)	0.0016 (7)
F2	0.0101 (7)	0.0284 (10)	0.0205 (9)	−0.0005 (6)	−0.0003 (6)	0.0023 (8)
F3	0.0170 (7)	0.0204 (9)	0.0163 (9)	0.0018 (7)	−0.0034 (6)	0.0024 (7)
C4	0.0098 (11)	0.0127 (13)	0.0193 (14)	−0.0006 (10)	−0.0004 (10)	−0.0018 (11)
C5	0.0172 (12)	0.0111 (13)	0.0155 (14)	−0.0027 (10)	0.0038 (11)	−0.0007 (11)
C6	0.0161 (12)	0.0118 (13)	0.0124 (13)	0.0014 (10)	−0.0043 (10)	−0.0012 (10)
C7	0.0118 (11)	0.0110 (13)	0.0191 (15)	0.0014 (10)	−0.0010 (10)	0.0000 (11)
C8	0.0141 (12)	0.0111 (13)	0.0148 (14)	0.0003 (10)	0.0033 (10)	−0.0016 (11)
C9	0.0137 (12)	0.0120 (13)	0.0153 (14)	0.0024 (10)	−0.0036 (10)	−0.0001 (11)
S1	0.0211 (3)	0.0144 (3)	0.0146 (3)	0.0003 (3)	0.0002 (3)	0.0002 (3)
N1	0.0236 (13)	0.0181 (13)	0.0267 (15)	−0.0027 (10)	0.0051 (11)	0.0020 (11)
N2	0.0321 (14)	0.0158 (13)	0.0292 (16)	0.0020 (11)	0.0127 (12)	0.0046 (12)
C1	0.0168 (13)	0.0223 (15)	0.0092 (14)	−0.0006 (11)	−0.0037 (10)	−0.0001 (11)
C2	0.0244 (14)	0.0209 (15)	0.0213 (16)	−0.0062 (12)	−0.0049 (12)	0.0046 (13)
C3	0.0397 (18)	0.0155 (15)	0.0278 (18)	0.0006 (14)	0.0044 (15)	0.0037 (13)

Geometric parameters (Å, º)

I1—C4	2.081 (2)	S1—C1	1.696 (3)
I2—C6	2.106 (3)	N1—HN1	0.831 (19)
I3—C8	2.100 (3)	N1—C1	1.326 (4)
F1—C5	1.349 (3)	N1—C2	1.460 (4)
F2—C7	1.356 (3)	N2—HN2	0.827 (18)
F3—C9	1.343 (3)	N2—C1	1.327 (4)
C4—C5	1.387 (4)	N2—C3	1.462 (4)
C4—C9	1.379 (4)	C2—H2A	0.9900
C5—C6	1.391 (4)	C2—H2B	0.9900
C6—C7	1.385 (4)	C2—C3	1.534 (4)
C7—C8	1.374 (4)	C3—H3A	0.9900
C8—C9	1.394 (4)	C3—H3B	0.9900
C5—C4—I1	121.0 (2)	C2—N1—HN1	128 (3)
C9—C4—I1	121.6 (2)	C1—N2—HN2	119 (3)
C9—C4—C5	117.4 (2)	C1—N2—C3	113.1 (3)
F1—C5—C4	118.7 (2)	C3—N2—HN2	127 (3)
F1—C5—C6	118.5 (3)	N1—C1—S1	125.4 (2)
C4—C5—C6	122.8 (3)	N1—C1—N2	108.7 (3)
C5—C6—I2	122.5 (2)	N2—C1—S1	125.9 (2)
C7—C6—I2	121.18 (19)	N1—C2—H2A	111.4
C7—C6—C5	116.3 (2)	N1—C2—H2B	111.4
F2—C7—C6	117.7 (2)	N1—C2—C3	102.1 (2)
F2—C7—C8	118.1 (2)	H2A—C2—H2B	109.2

C8—C7—C6	124.2 (2)	C3—C2—H2A	111.4
C7—C8—I3	122.51 (19)	C3—C2—H2B	111.4
C7—C8—C9	116.4 (3)	N2—C3—C2	102.3 (3)
C9—C8—I3	121.0 (2)	N2—C3—H3A	111.3
F3—C9—C4	118.7 (2)	N2—C3—H3B	111.3
F3—C9—C8	118.3 (2)	C2—C3—H3A	111.3
C4—C9—C8	122.9 (3)	C2—C3—H3B	111.3
C1—N1—HN1	118 (3)	H3A—C3—H3B	109.2
C1—N1—C2	113.5 (3)		

I1—C4—C5—F1	−0.2 (3)	C5—C6—C7—F2	−179.8 (2)
I1—C4—C5—C6	179.3 (2)	C5—C6—C7—C8	1.1 (4)
I1—C4—C9—F3	1.7 (4)	C6—C7—C8—I3	−177.9 (2)
I1—C4—C9—C8	−178.1 (2)	C6—C7—C8—C9	0.1 (4)
I2—C6—C7—F2	1.9 (3)	C7—C8—C9—F3	179.0 (2)
I2—C6—C7—C8	−177.3 (2)	C7—C8—C9—C4	−1.2 (4)
I3—C8—C9—F3	−2.9 (3)	C9—C4—C5—F1	−179.2 (2)
I3—C8—C9—C4	176.8 (2)	C9—C4—C5—C6	0.2 (4)
F1—C5—C6—I2	−3.4 (4)	N1—C2—C3—N2	5.8 (3)
F1—C5—C6—C7	178.2 (2)	C1—N1—C2—C3	−3.7 (3)
F2—C7—C8—I3	2.9 (4)	C1—N2—C3—C2	−6.8 (4)
F2—C7—C8—C9	−179.1 (2)	C2—N1—C1—S1	−179.8 (2)
C4—C5—C6—I2	177.1 (2)	C2—N1—C1—N2	−0.4 (4)
C4—C5—C6—C7	−1.2 (4)	C3—N2—C1—S1	−175.8 (2)
C5—C4—C9—F3	−179.2 (2)	C3—N2—C1—N1	4.8 (4)
C5—C4—C9—C8	1.0 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H*N*2···I2^{i}	0.83 (2)	3.10 (3)	3.742 (3)	137 (3)
C2—H2*B*···I1^{ii}	0.99	3.31	3.927 (3)	122
C2—H2*B*···F3^{iii}	0.99	2.47	3.147 (3)	125

Symmetry codes: (i) −*x*+3/2, *y*+1/2, *z*; (ii) −*x*+1, *y*−1/2, −*z*+3/2; (iii) *x*, −*y*+1/2, *z*+1/2.

1*H*-1,3-Benzodiazole-2-thiol–1,2,3,5-tetrafluoro-4,6-diiodobenzene (4/3) (4MBZIM_313F4DIB)

Crystal data

$3C_6F_4I_2·4C_7H_6N_2S$
M_r = 1806.37
Triclinic, $P\overline{1}$
a = 8.4573 (14) Å
b = 17.725 (3) Å
c = 18.759 (4) Å
α = 106.997 (7)°
β = 93.229 (7)°
γ = 92.034 (7)°
V = 2680.9 (9) Å^3

Z = 2
F(000) = 1692
D_x = 2.238 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 9879 reflections
θ = 2.4–27.5°
μ = 3.72 mm^{-1}
T = 100 K
Needle, colourless
0.34 × 0.04 × 0.04 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec IμS
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.668, T_{max} = 0.746
118524 measured reflections
12297 independent reflections
10558 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 27.6°, θ_{min} = 2.2°
h = −10→10
k = −23→23
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.041
S = 1.06
12297 reflections
717 parameters
8 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0068P)^2 + 2.3276P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.75 e Å^{-3}

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.

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

	x	y	z	U_{iso}*/U_{eq}
I1	0.23723 (2)	0.28696 (2)	0.64287 (2)	0.01892 (4)
I2	0.11203 (2)	0.62311 (2)	0.81696 (2)	0.02185 (4)
F29	0.12514 (17)	0.43584 (9)	0.76730 (8)	0.0228 (3)
F30	0.28968 (19)	0.64658 (9)	0.67800 (9)	0.0259 (3)
F31	0.41295 (19)	0.54429 (9)	0.56177 (9)	0.0271 (4)
F32	0.38986 (17)	0.38762 (9)	0.54469 (8)	0.0234 (3)
C29	0.2585 (3)	0.40830 (15)	0.65651 (14)	0.0161 (5)
C30	0.1965 (3)	0.46280 (16)	0.71636 (14)	0.0182 (5)
C31	0.2045 (3)	0.54314 (15)	0.72577 (14)	0.0166 (5)
C32	0.2787 (3)	0.56938 (15)	0.67263 (14)	0.0186 (5)
C33	0.3417 (3)	0.51713 (16)	0.61237 (14)	0.0193 (5)
C34	0.3307 (3)	0.43733 (16)	0.60458 (14)	0.0183 (5)
I3	0.39366 (2)	0.29864 (2)	0.15711 (2)	0.02594 (4)
I4	0.19057 (2)	0.58106 (2)	0.39910 (2)	0.02628 (4)
F33	0.31982 (19)	0.47479 (9)	0.24734 (9)	0.0278 (4)
F34	0.11956 (18)	0.43808 (10)	0.46524 (9)	0.0290 (4)
F35	0.17740 (18)	0.28360 (10)	0.41706 (9)	0.0295 (4)
F36	0.30202 (17)	0.22313 (9)	0.28451 (9)	0.0256 (3)
C35	0.2209 (3)	0.46038 (15)	0.35750 (15)	0.0190 (5)
C36	0.2842 (3)	0.42746 (16)	0.28917 (14)	0.0191 (5)
C37	0.3114 (3)	0.34781 (15)	0.26241 (14)	0.0178 (5)

C38	0.2759 (3)	0.30052 (15)	0.30711 (15)	0.0192 (5)
C39	0.2115 (3)	0.33102 (16)	0.37517 (15)	0.0210 (6)
C40	0.1836 (3)	0.40999 (16)	0.39927 (14)	0.0200 (5)
I5	0.82526 (2)	0.39902 (2)	−0.11345 (2)	0.02532 (4)
I6	0.75419 (2)	0.73973 (2)	0.07191 (2)	0.01718 (4)
F37	0.85766 (18)	0.58847 (9)	−0.05559 (8)	0.0244 (3)
F38	0.59562 (17)	0.64129 (9)	0.16783 (8)	0.0218 (3)
F39	0.54190 (18)	0.48581 (9)	0.14581 (9)	0.0262 (4)
F40	0.63996 (18)	0.38040 (9)	0.02360 (9)	0.0255 (3)
C41	0.7536 (3)	0.48240 (15)	−0.01841 (14)	0.0169 (5)
C42	0.7782 (3)	0.56261 (15)	−0.00623 (14)	0.0164 (5)
C43	0.7249 (3)	0.61822 (14)	0.05532 (14)	0.0149 (5)
C44	0.6468 (3)	0.59054 (15)	0.10618 (14)	0.0168 (5)
C45	0.6198 (3)	0.51085 (15)	0.09575 (14)	0.0180 (5)
C46	0.6721 (3)	0.45764 (15)	0.03328 (15)	0.0182 (5)
S1	1.26980 (7)	0.02971 (4)	0.13364 (4)	0.01658 (13)
N1	1.3937 (2)	−0.08314 (13)	0.19002 (11)	0.0155 (4)
HN1	1.487 (2)	−0.0747 (18)	0.1788 (17)	0.031 (9)*
N2	1.1363 (2)	−0.08180 (12)	0.18912 (11)	0.0153 (4)
HN2	1.041 (2)	−0.0708 (15)	0.1806 (14)	0.015 (7)*
C1	1.2668 (3)	−0.04645 (15)	0.17100 (13)	0.0158 (5)
C2	1.3451 (3)	−0.14290 (15)	0.21949 (13)	0.0154 (5)
C3	1.4285 (3)	−0.19430 (15)	0.24861 (14)	0.0188 (5)
H3	1.540814	−0.194912	0.248974	0.023*
C4	1.3406 (3)	−0.24474 (16)	0.27716 (14)	0.0208 (6)
H4	1.393923	−0.280671	0.297743	0.025*
C5	1.1748 (3)	−0.24408 (16)	0.27645 (14)	0.0197 (5)
H5	1.118578	−0.279849	0.296263	0.024*
C6	1.0905 (3)	−0.19247 (15)	0.24751 (14)	0.0182 (5)
H6	0.978144	−0.191915	0.247143	0.022*
C7	1.1792 (3)	−0.14174 (15)	0.21913 (13)	0.0159 (5)
S2	0.76230 (7)	−0.07080 (4)	0.13517 (3)	0.01460 (12)
N3	0.8902 (2)	0.04164 (12)	0.07893 (12)	0.0142 (4)
HN3	0.985 (2)	0.0339 (17)	0.0913 (16)	0.026 (8)*
N4	0.6315 (2)	0.03610 (12)	0.07390 (11)	0.0134 (4)
HN4	0.539 (2)	0.0257 (15)	0.0851 (15)	0.016 (7)*
C8	0.7619 (3)	0.00336 (14)	0.09496 (13)	0.0135 (5)
C9	0.8425 (3)	0.10176 (14)	0.04983 (13)	0.0149 (5)
C10	0.9275 (3)	0.15703 (15)	0.02577 (14)	0.0186 (5)
H10	1.040174	0.160378	0.028830	0.022*
C11	0.8386 (3)	0.20721 (15)	−0.00307 (15)	0.0199 (5)
H11	0.892259	0.246317	−0.019649	0.024*
C12	0.6733 (3)	0.20197 (15)	−0.00842 (14)	0.0185 (5)
H12	0.617475	0.236637	−0.029681	0.022*
C13	0.5882 (3)	0.14726 (15)	0.01657 (13)	0.0160 (5)
H13	0.475508	0.143780	0.013282	0.019*
C14	0.6767 (3)	0.09798 (14)	0.04661 (13)	0.0137 (5)
S3	0.21077 (7)	1.09011 (4)	0.59658 (4)	0.01674 (13)

N5	0.3335 (2)	0.98621 (12)	0.66496 (12)	0.0153 (4)
HN5	0.427 (2)	0.9957 (18)	0.6541 (17)	0.035 (9)*
N6	0.0755 (2)	0.98679 (12)	0.66091 (12)	0.0149 (4)
HN6	−0.020 (2)	0.9958 (16)	0.6501 (15)	0.021 (8)*
C15	0.2063 (3)	1.02032 (14)	0.64225 (13)	0.0147 (5)
C16	0.2825 (3)	0.92908 (14)	0.69697 (13)	0.0149 (5)
C17	0.3645 (3)	0.87884 (15)	0.72898 (14)	0.0196 (5)
H17	0.477019	0.878891	0.731657	0.024*
C18	0.2730 (3)	0.82880 (15)	0.75670 (14)	0.0211 (6)
H18	0.324318	0.793463	0.778775	0.025*
C19	0.1078 (3)	0.82884 (15)	0.75312 (14)	0.0213 (6)
H19	0.049812	0.793080	0.772293	0.026*
C20	0.0256 (3)	0.87954 (15)	0.72240 (14)	0.0186 (5)
H20	−0.086842	0.880244	0.720810	0.022*
C21	0.1171 (3)	0.92909 (14)	0.69418 (13)	0.0141 (5)
S4	−0.29930 (7)	0.99445 (4)	0.61172 (3)	0.01608 (12)
N7	−0.1672 (2)	1.09905 (13)	0.54729 (12)	0.0157 (4)
HN7	−0.073 (2)	1.0901 (18)	0.5580 (17)	0.033 (9)*
N8	−0.4249 (2)	1.09692 (13)	0.54319 (12)	0.0156 (4)
HN8	−0.519 (2)	1.0848 (17)	0.5511 (17)	0.029 (8)*
C22	−0.2972 (3)	1.06481 (14)	0.56708 (13)	0.0146 (5)
C23	−0.2121 (3)	1.15416 (14)	0.51139 (13)	0.0145 (5)
C24	−0.1251 (3)	1.20294 (15)	0.48049 (14)	0.0186 (5)
H24	−0.012656	1.203249	0.481615	0.022*
C25	−0.2099 (3)	1.25129 (15)	0.44782 (14)	0.0189 (5)
H25	−0.154262	1.285731	0.426292	0.023*
C26	−0.3758 (3)	1.25043 (15)	0.44591 (14)	0.0189 (5)
H26	−0.429872	1.284470	0.423194	0.023*
C27	−0.4633 (3)	1.20121 (15)	0.47629 (14)	0.0185 (5)
H27	−0.575825	1.200557	0.474834	0.022*
C28	−0.3778 (3)	1.15290 (14)	0.50896 (13)	0.0147 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01909 (8)	0.01702 (9)	0.02029 (9)	0.00047 (6)	−0.00052 (6)	0.00538 (7)
I2	0.02488 (9)	0.02320 (9)	0.01763 (9)	0.00734 (7)	0.00435 (7)	0.00505 (7)
F29	0.0267 (8)	0.0243 (9)	0.0207 (8)	0.0015 (6)	0.0077 (6)	0.0105 (7)
F30	0.0389 (9)	0.0165 (8)	0.0242 (9)	0.0008 (7)	0.0055 (7)	0.0085 (7)
F31	0.0365 (9)	0.0267 (9)	0.0217 (8)	−0.0001 (7)	0.0121 (7)	0.0112 (7)
F32	0.0259 (8)	0.0241 (9)	0.0192 (8)	0.0051 (6)	0.0067 (6)	0.0034 (7)
C29	0.0157 (12)	0.0150 (13)	0.0176 (13)	0.0003 (9)	−0.0012 (9)	0.0052 (11)
C30	0.0148 (12)	0.0233 (14)	0.0179 (13)	0.0010 (10)	0.0011 (10)	0.0080 (11)
C31	0.0165 (12)	0.0192 (14)	0.0134 (12)	0.0051 (10)	0.0015 (9)	0.0035 (10)
C32	0.0210 (13)	0.0174 (14)	0.0185 (13)	0.0012 (10)	−0.0005 (10)	0.0074 (11)
C33	0.0193 (13)	0.0244 (15)	0.0167 (13)	0.0000 (10)	0.0034 (10)	0.0098 (11)
C34	0.0151 (12)	0.0228 (14)	0.0154 (13)	0.0019 (10)	0.0009 (9)	0.0030 (11)
I3	0.03176 (10)	0.02680 (10)	0.01832 (9)	0.00506 (7)	0.00720 (7)	0.00377 (8)

I4	0.02547 (9)	0.01905 (9)	0.02967 (10)	0.00413 (7)	−0.00068 (7)	0.00011 (8)
F33	0.0386 (9)	0.0238 (9)	0.0252 (9)	0.0027 (7)	0.0080 (7)	0.0127 (7)
F34	0.0306 (9)	0.0367 (10)	0.0183 (8)	0.0053 (7)	0.0094 (7)	0.0040 (7)
F35	0.0325 (9)	0.0313 (10)	0.0308 (9)	−0.0031 (7)	0.0084 (7)	0.0182 (8)
F36	0.0261 (8)	0.0155 (8)	0.0351 (10)	0.0008 (6)	0.0060 (7)	0.0067 (7)
C35	0.0159 (12)	0.0174 (14)	0.0218 (14)	0.0018 (10)	−0.0004 (10)	0.0029 (11)
C36	0.0178 (12)	0.0221 (14)	0.0190 (13)	−0.0006 (10)	−0.0005 (10)	0.0090 (11)
C37	0.0169 (12)	0.0206 (14)	0.0149 (13)	0.0025 (10)	0.0004 (9)	0.0035 (11)
C38	0.0142 (12)	0.0180 (14)	0.0243 (14)	0.0006 (10)	−0.0012 (10)	0.0048 (11)
C39	0.0181 (13)	0.0272 (15)	0.0201 (14)	−0.0035 (10)	0.0008 (10)	0.0116 (12)
C40	0.0159 (12)	0.0275 (15)	0.0151 (13)	0.0007 (10)	0.0017 (10)	0.0039 (11)
I5	0.02794 (9)	0.02317 (10)	0.01987 (9)	0.00810 (7)	0.00031 (7)	−0.00193 (7)
I6	0.01777 (8)	0.01347 (8)	0.02020 (9)	−0.00095 (6)	−0.00012 (6)	0.00532 (7)
F37	0.0293 (8)	0.0248 (9)	0.0215 (8)	0.0003 (7)	0.0103 (6)	0.0092 (7)
F38	0.0267 (8)	0.0201 (8)	0.0186 (8)	0.0047 (6)	0.0078 (6)	0.0039 (7)
F39	0.0332 (9)	0.0240 (9)	0.0274 (9)	0.0000 (7)	0.0085 (7)	0.0158 (7)
F40	0.0338 (9)	0.0131 (8)	0.0291 (9)	−0.0013 (6)	−0.0028 (7)	0.0066 (7)
C41	0.0172 (12)	0.0161 (13)	0.0151 (13)	0.0049 (10)	−0.0016 (9)	0.0011 (10)
C42	0.0149 (12)	0.0198 (14)	0.0155 (13)	0.0007 (10)	0.0013 (9)	0.0064 (11)
C43	0.0149 (12)	0.0125 (12)	0.0174 (13)	0.0015 (9)	−0.0011 (9)	0.0049 (10)
C44	0.0162 (12)	0.0176 (13)	0.0161 (13)	0.0027 (10)	0.0006 (9)	0.0041 (11)
C45	0.0182 (12)	0.0182 (14)	0.0195 (13)	−0.0002 (10)	0.0004 (10)	0.0090 (11)
C46	0.0213 (13)	0.0106 (13)	0.0217 (14)	−0.0014 (10)	−0.0053 (10)	0.0050 (11)
S1	0.0117 (3)	0.0187 (3)	0.0194 (3)	0.0011 (2)	0.0010 (2)	0.0057 (3)
N1	0.0100 (10)	0.0206 (12)	0.0150 (11)	0.0013 (8)	0.0013 (8)	0.0037 (9)
N2	0.0094 (10)	0.0198 (12)	0.0169 (11)	0.0021 (8)	0.0008 (8)	0.0057 (9)
C1	0.0141 (12)	0.0179 (13)	0.0123 (12)	0.0001 (9)	0.0015 (9)	−0.0002 (10)
C2	0.0142 (12)	0.0165 (13)	0.0125 (12)	0.0001 (9)	−0.0003 (9)	0.0001 (10)
C3	0.0141 (12)	0.0223 (14)	0.0182 (13)	0.0028 (10)	0.0003 (10)	0.0029 (11)
C4	0.0229 (13)	0.0214 (14)	0.0178 (13)	0.0037 (11)	−0.0007 (10)	0.0052 (11)
C5	0.0235 (13)	0.0191 (14)	0.0148 (13)	−0.0021 (10)	0.0026 (10)	0.0026 (11)
C6	0.0163 (12)	0.0203 (14)	0.0157 (13)	−0.0001 (10)	0.0015 (10)	0.0019 (11)
C7	0.0165 (12)	0.0174 (13)	0.0127 (12)	0.0013 (10)	−0.0010 (9)	0.0029 (10)
S2	0.0118 (3)	0.0130 (3)	0.0192 (3)	0.0003 (2)	0.0004 (2)	0.0054 (3)
N3	0.0096 (10)	0.0158 (11)	0.0180 (11)	0.0016 (8)	0.0003 (8)	0.0061 (9)
N4	0.0112 (10)	0.0133 (11)	0.0153 (11)	0.0011 (8)	0.0004 (8)	0.0036 (9)
C8	0.0126 (11)	0.0128 (12)	0.0127 (12)	0.0017 (9)	0.0000 (9)	0.0004 (10)
C9	0.0154 (12)	0.0147 (13)	0.0138 (12)	0.0003 (9)	0.0011 (9)	0.0030 (10)
C10	0.0148 (12)	0.0200 (14)	0.0208 (14)	−0.0018 (10)	0.0018 (10)	0.0058 (11)
C11	0.0216 (13)	0.0173 (14)	0.0221 (14)	−0.0012 (10)	0.0041 (10)	0.0079 (11)
C12	0.0231 (13)	0.0154 (13)	0.0167 (13)	0.0030 (10)	−0.0006 (10)	0.0045 (11)
C13	0.0146 (12)	0.0164 (13)	0.0147 (12)	0.0044 (9)	0.0019 (9)	0.0003 (10)
C14	0.0143 (11)	0.0126 (12)	0.0132 (12)	−0.0006 (9)	0.0027 (9)	0.0022 (10)
S3	0.0129 (3)	0.0165 (3)	0.0224 (3)	0.0008 (2)	0.0024 (2)	0.0079 (3)
N5	0.0123 (10)	0.0155 (11)	0.0178 (11)	0.0017 (8)	0.0011 (8)	0.0042 (9)
N6	0.0103 (10)	0.0145 (11)	0.0194 (11)	0.0007 (8)	0.0007 (8)	0.0043 (9)
C15	0.0139 (11)	0.0145 (13)	0.0142 (12)	0.0017 (9)	0.0023 (9)	0.0015 (10)
C16	0.0165 (12)	0.0135 (13)	0.0118 (12)	0.0002 (9)	−0.0012 (9)	−0.0005 (10)

C17	0.0189 (13)	0.0204 (14)	0.0163 (13)	0.0065 (10)	−0.0022 (10)	0.0003 (11)
C18	0.0306 (14)	0.0167 (14)	0.0141 (13)	0.0056 (11)	−0.0041 (10)	0.0022 (11)
C19	0.0300 (14)	0.0166 (14)	0.0179 (14)	−0.0005 (11)	0.0020 (11)	0.0063 (11)
C20	0.0206 (13)	0.0167 (13)	0.0165 (13)	−0.0009 (10)	0.0015 (10)	0.0020 (11)
C21	0.0158 (12)	0.0137 (12)	0.0108 (12)	0.0019 (9)	−0.0008 (9)	0.0007 (10)
S4	0.0130 (3)	0.0184 (3)	0.0182 (3)	−0.0002 (2)	0.0001 (2)	0.0078 (3)
N7	0.0114 (10)	0.0195 (12)	0.0159 (11)	−0.0007 (8)	−0.0008 (8)	0.0054 (9)
N8	0.0111 (10)	0.0199 (12)	0.0168 (11)	−0.0001 (8)	0.0016 (8)	0.0070 (9)
C22	0.0146 (12)	0.0152 (13)	0.0119 (12)	0.0007 (9)	−0.0003 (9)	0.0007 (10)
C23	0.0166 (12)	0.0127 (12)	0.0110 (12)	0.0000 (9)	0.0001 (9)	−0.0011 (10)
C24	0.0182 (12)	0.0192 (14)	0.0164 (13)	−0.0050 (10)	0.0018 (10)	0.0028 (11)
C25	0.0254 (13)	0.0141 (13)	0.0169 (13)	−0.0022 (10)	0.0030 (10)	0.0044 (11)
C26	0.0242 (13)	0.0166 (13)	0.0153 (13)	0.0017 (10)	0.0009 (10)	0.0037 (11)
C27	0.0164 (12)	0.0191 (14)	0.0187 (13)	0.0018 (10)	0.0005 (10)	0.0035 (11)
C28	0.0162 (12)	0.0134 (12)	0.0143 (12)	−0.0012 (9)	0.0016 (9)	0.0037 (10)

Geometric parameters (Å, º)

I1—C29	2.090 (3)	C6—C7	1.390 (3)
I2—C31	2.088 (2)	S2—C8	1.696 (2)
F29—C30	1.348 (3)	N3—HN3	0.846 (17)
F30—C32	1.342 (3)	N3—C8	1.354 (3)
F31—C33	1.344 (3)	N3—C9	1.394 (3)
F32—C34	1.343 (3)	N4—HN4	0.849 (16)
C29—C30	1.392 (3)	N4—C8	1.356 (3)
C29—C34	1.387 (3)	N4—C14	1.390 (3)
C30—C31	1.382 (4)	C9—C10	1.388 (3)
C31—C32	1.387 (3)	C9—C14	1.398 (3)
C32—C33	1.382 (4)	C10—H10	0.9500
C33—C34	1.378 (4)	C10—C11	1.390 (3)
I3—C37	2.083 (2)	C11—H11	0.9500
I4—C35	2.082 (3)	C11—C12	1.394 (3)
F33—C36	1.343 (3)	C12—H12	0.9500
F34—C40	1.344 (3)	C12—C13	1.391 (4)
F35—C39	1.342 (3)	C13—H13	0.9500
F36—C38	1.342 (3)	C13—C14	1.388 (3)
C35—C36	1.390 (4)	S3—C15	1.699 (2)
C35—C40	1.389 (4)	N5—HN5	0.850 (17)
C36—C37	1.386 (4)	N5—C15	1.360 (3)
C37—C38	1.385 (4)	N5—C16	1.388 (3)
C38—C39	1.383 (4)	N6—HN6	0.851 (17)
C39—C40	1.373 (4)	N6—C15	1.348 (3)
I5—C41	2.092 (2)	N6—C21	1.390 (3)
I6—C43	2.088 (2)	C16—C17	1.394 (3)
F37—C42	1.347 (3)	C16—C21	1.398 (3)
F38—C44	1.345 (3)	C17—H17	0.9500
F39—C45	1.344 (3)	C17—C18	1.386 (4)
F40—C46	1.343 (3)	C18—H18	0.9500

C41—C42	1.379 (4)	C18—C19	1.396 (4)
C41—C46	1.382 (4)	C19—H19	0.9500
C42—C43	1.390 (3)	C19—C20	1.387 (3)
C43—C44	1.382 (3)	C20—H20	0.9500
C44—C45	1.377 (4)	C20—C21	1.386 (3)
C45—C46	1.378 (4)	S4—C22	1.693 (2)
S1—C1	1.693 (3)	N7—HN7	0.844 (17)
N1—HN1	0.847 (17)	N7—C22	1.358 (3)
N1—C1	1.358 (3)	N7—C23	1.391 (3)
N1—C2	1.390 (3)	N8—HN8	0.852 (17)
N2—HN2	0.854 (16)	N8—C22	1.353 (3)
N2—C1	1.358 (3)	N8—C28	1.389 (3)
N2—C7	1.390 (3)	C23—C24	1.386 (3)
C2—C3	1.385 (3)	C23—C28	1.398 (3)
C2—C7	1.404 (3)	C24—H24	0.9500
C3—H3	0.9500	C24—C25	1.388 (3)
C3—C4	1.384 (4)	C25—H25	0.9500
C4—H4	0.9500	C25—C26	1.401 (3)
C4—C5	1.402 (3)	C26—H26	0.9500
C5—H5	0.9500	C26—C27	1.388 (4)
C5—C6	1.390 (3)	C27—H27	0.9500
C6—H6	0.9500	C27—C28	1.390 (3)

C30—C29—I1	121.55 (18)	C8—N3—HN3	123 (2)
C34—C29—I1	120.98 (19)	C8—N3—C9	110.03 (19)
C34—C29—C30	117.4 (2)	C9—N3—HN3	126 (2)
F29—C30—C29	118.4 (2)	C8—N4—HN4	122.6 (18)
F29—C30—C31	118.6 (2)	C8—N4—C14	109.91 (19)
C31—C30—C29	123.0 (2)	C14—N4—HN4	126.3 (18)
C30—C31—I2	121.81 (18)	N3—C8—S2	126.82 (17)
C30—C31—C32	117.5 (2)	N3—C8—N4	107.3 (2)
C32—C31—I2	120.72 (19)	N4—C8—S2	125.90 (18)
F30—C32—C31	120.7 (2)	N3—C9—C14	106.2 (2)
F30—C32—C33	118.0 (2)	C10—C9—N3	132.1 (2)
C33—C32—C31	121.3 (2)	C10—C9—C14	121.7 (2)
F31—C33—C32	120.0 (2)	C9—C10—H10	121.9
F31—C33—C34	120.4 (2)	C9—C10—C11	116.3 (2)
C34—C33—C32	119.6 (2)	C11—C10—H10	121.9
F32—C34—C29	120.3 (2)	C10—C11—H11	119.0
F32—C34—C33	118.5 (2)	C10—C11—C12	122.1 (2)
C33—C34—C29	121.2 (2)	C12—C11—H11	119.0
C36—C35—I4	122.13 (19)	C11—C12—H12	119.2
C40—C35—I4	120.40 (19)	C13—C12—C11	121.6 (2)
C40—C35—C36	117.4 (2)	C13—C12—H12	119.2
F33—C36—C35	118.6 (2)	C12—C13—H13	121.8
F33—C36—C37	118.7 (2)	C14—C13—C12	116.4 (2)
C37—C36—C35	122.7 (2)	C14—C13—H13	121.8
C36—C37—I3	121.94 (19)	N4—C14—C9	106.5 (2)

C38—C37—I3	120.42 (19)	C13—C14—N4	131.5 (2)
C38—C37—C36	117.6 (2)	C13—C14—C9	121.9 (2)
F36—C38—C37	120.2 (2)	C15—N5—HN5	122 (2)
F36—C38—C39	118.4 (2)	C15—N5—C16	109.8 (2)
C39—C38—C37	121.4 (2)	C16—N5—HN5	128 (2)
F35—C39—C38	120.0 (2)	C15—N6—HN6	125.4 (19)
F35—C39—C40	120.6 (2)	C15—N6—C21	110.28 (19)
C40—C39—C38	119.4 (2)	C21—N6—HN6	124.0 (19)
F34—C40—C35	120.2 (2)	N5—C15—S3	126.48 (18)
F34—C40—C39	118.3 (2)	N6—C15—S3	126.32 (18)
C39—C40—C35	121.5 (2)	N6—C15—N5	107.2 (2)
C42—C41—I5	122.49 (18)	N5—C16—C17	132.2 (2)
C42—C41—C46	117.7 (2)	N5—C16—C21	106.5 (2)
C46—C41—I5	119.79 (19)	C17—C16—C21	121.2 (2)
F37—C42—C41	119.0 (2)	C16—C17—H17	121.8
F37—C42—C43	118.4 (2)	C18—C17—C16	116.4 (2)
C41—C42—C43	122.6 (2)	C18—C17—H17	121.8
C42—C43—I6	122.78 (18)	C17—C18—H18	119.1
C44—C43—I6	119.64 (18)	C17—C18—C19	121.9 (2)
C44—C43—C42	117.6 (2)	C19—C18—H18	119.1
F38—C44—C43	120.5 (2)	C18—C19—H19	119.0
F38—C44—C45	118.2 (2)	C20—C19—C18	122.0 (2)
C45—C44—C43	121.4 (2)	C20—C19—H19	119.0
F39—C45—C44	120.0 (2)	C19—C20—H20	122.0
F39—C45—C46	120.8 (2)	C21—C20—C19	116.1 (2)
C44—C45—C46	119.3 (2)	C21—C20—H20	122.0
F40—C46—C41	120.7 (2)	N6—C21—C16	106.2 (2)
F40—C46—C45	117.8 (2)	C20—C21—N6	131.4 (2)
C45—C46—C41	121.5 (2)	C20—C21—C16	122.4 (2)
C1—N1—HN1	123 (2)	C22—N7—HN7	124 (2)
C1—N1—C2	110.7 (2)	C22—N7—C23	110.29 (19)
C2—N1—HN1	126 (2)	C23—N7—HN7	125 (2)
C1—N2—HN2	124.7 (18)	C22—N8—HN8	122 (2)
C1—N2—C7	110.48 (19)	C22—N8—C28	110.6 (2)
C7—N2—HN2	124.7 (18)	C28—N8—HN8	127 (2)
N1—C1—S1	127.03 (19)	N7—C22—S4	126.72 (18)
N1—C1—N2	106.5 (2)	N8—C22—S4	126.58 (18)
N2—C1—S1	126.41 (18)	N8—C22—N7	106.7 (2)
N1—C2—C7	106.0 (2)	N7—C23—C28	106.2 (2)
C3—C2—N1	132.4 (2)	C24—C23—N7	132.1 (2)
C3—C2—C7	121.6 (2)	C24—C23—C28	121.6 (2)
C2—C3—H3	121.5	C23—C24—H24	121.5
C4—C3—C2	116.9 (2)	C23—C24—C25	116.9 (2)
C4—C3—H3	121.5	C25—C24—H24	121.5
C3—C4—H4	119.2	C24—C25—H25	119.3
C3—C4—C5	121.6 (2)	C24—C25—C26	121.4 (2)
C5—C4—H4	119.2	C26—C25—H25	119.3
C4—C5—H5	119.1	C25—C26—H26	119.1

C6—C5—C4	121.8 (2)	C27—C26—C25	121.8 (2)
C6—C5—H5	119.1	C27—C26—H26	119.1
C5—C6—H6	121.8	C26—C27—H27	121.7
C7—C6—C5	116.5 (2)	C26—C27—C28	116.5 (2)
C7—C6—H6	121.8	C28—C27—H27	121.7
N2—C7—C2	106.3 (2)	N8—C28—C23	106.2 (2)
N2—C7—C6	132.0 (2)	N8—C28—C27	132.1 (2)
C6—C7—C2	121.6 (2)	C27—C28—C23	121.7 (2)
I1—C29—C30—F29	1.8 (3)	N1—C2—C7—C6	−177.7 (2)
I1—C29—C30—C31	−178.02 (18)	C1—N1—C2—C3	−177.6 (3)
I1—C29—C34—F32	−0.7 (3)	C1—N1—C2—C7	−0.7 (3)
I1—C29—C34—C33	178.45 (19)	C1—N2—C7—C2	0.1 (3)
I2—C31—C32—F30	−1.4 (3)	C1—N2—C7—C6	177.9 (3)
I2—C31—C32—C33	179.38 (19)	C2—N1—C1—S1	179.67 (19)
F29—C30—C31—I2	0.8 (3)	C2—N1—C1—N2	0.8 (3)
F29—C30—C31—C32	179.9 (2)	C2—C3—C4—C5	0.2 (4)
F30—C32—C33—F31	0.7 (4)	C3—C2—C7—N2	177.6 (2)
F30—C32—C33—C34	−179.2 (2)	C3—C2—C7—C6	−0.5 (4)
F31—C33—C34—F32	−1.3 (4)	C3—C4—C5—C6	−0.4 (4)
F31—C33—C34—C29	179.6 (2)	C4—C5—C6—C7	0.2 (4)
C29—C30—C31—I2	−179.37 (18)	C5—C6—C7—N2	−177.3 (3)
C29—C30—C31—C32	−0.3 (4)	C5—C6—C7—C2	0.2 (4)
C30—C29—C34—F32	−178.6 (2)	C7—N2—C1—S1	−179.44 (19)
C30—C29—C34—C33	0.5 (4)	C7—N2—C1—N1	−0.6 (3)
C30—C31—C32—F30	179.5 (2)	C7—C2—C3—C4	0.2 (4)
C30—C31—C32—C33	0.3 (4)	N3—C9—C10—C11	177.7 (3)
C31—C32—C33—F31	180.0 (2)	N3—C9—C14—N4	0.1 (3)
C31—C32—C33—C34	0.1 (4)	N3—C9—C14—C13	−176.7 (2)
C32—C33—C34—F32	178.6 (2)	C8—N3—C9—C10	179.5 (3)
C32—C33—C34—C29	−0.5 (4)	C8—N3—C9—C14	−1.5 (3)
C34—C29—C30—F29	179.7 (2)	C8—N4—C14—C9	1.3 (3)
C34—C29—C30—C31	−0.1 (4)	C8—N4—C14—C13	177.6 (3)
I3—C37—C38—F36	3.5 (3)	C9—N3—C8—S2	−176.81 (19)
I3—C37—C38—C39	−175.80 (19)	C9—N3—C8—N4	2.3 (3)
I4—C35—C36—F33	−3.1 (3)	C9—C10—C11—C12	−0.7 (4)
I4—C35—C36—C37	177.10 (19)	C10—C9—C14—N4	179.3 (2)
I4—C35—C40—F34	3.5 (3)	C10—C9—C14—C13	2.5 (4)
I4—C35—C40—C39	−175.96 (19)	C10—C11—C12—C13	1.6 (4)
F33—C36—C37—I3	−3.5 (3)	C11—C12—C13—C14	−0.4 (4)
F33—C36—C37—C38	179.1 (2)	C12—C13—C14—N4	−177.5 (2)
F35—C39—C40—F34	−0.8 (4)	C12—C13—C14—C9	−1.6 (4)
F35—C39—C40—C35	178.7 (2)	C14—N4—C8—S2	176.89 (18)
F36—C38—C39—F35	0.3 (4)	C14—N4—C8—N3	−2.2 (3)
F36—C38—C39—C40	−179.9 (2)	C14—C9—C10—C11	−1.3 (4)
C35—C36—C37—I3	176.28 (19)	N5—C16—C17—C18	179.3 (3)
C35—C36—C37—C38	−1.2 (4)	N5—C16—C21—N6	−0.4 (3)
C36—C35—C40—F34	−178.9 (2)	N5—C16—C21—C20	−179.2 (2)

C36—C35—C40—C39	1.6 (4)	C15—N5—C16—C17	−179.3 (3)
C36—C37—C38—F36	−179.0 (2)	C15—N5—C16—C21	−0.6 (3)
C36—C37—C38—C39	1.7 (4)	C15—N6—C21—C16	1.2 (3)
C37—C38—C39—F35	179.6 (2)	C15—N6—C21—C20	179.8 (3)
C37—C38—C39—C40	−0.6 (4)	C16—N5—C15—S3	−177.01 (19)
C38—C39—C40—F34	179.4 (2)	C16—N5—C15—N6	1.3 (3)
C38—C39—C40—C35	−1.1 (4)	C16—C17—C18—C19	−0.3 (4)
C40—C35—C36—F33	179.3 (2)	C17—C16—C21—N6	178.5 (2)
C40—C35—C36—C37	−0.4 (4)	C17—C16—C21—C20	−0.3 (4)
I5—C41—C42—F37	−3.0 (3)	C17—C18—C19—C20	−0.7 (4)
I5—C41—C42—C43	177.25 (18)	C18—C19—C20—C21	1.2 (4)
I5—C41—C46—F40	0.8 (3)	C19—C20—C21—N6	−179.1 (2)
I5—C41—C46—C45	−178.55 (18)	C19—C20—C21—C16	−0.7 (4)
I6—C43—C44—F38	−2.9 (3)	C21—N6—C15—S3	176.77 (19)
I6—C43—C44—C45	177.54 (18)	C21—N6—C15—N5	−1.6 (3)
F37—C42—C43—I6	2.7 (3)	C21—C16—C17—C18	0.8 (4)
F37—C42—C43—C44	−178.6 (2)	N7—C23—C24—C25	179.5 (2)
F38—C44—C45—F39	1.2 (3)	N7—C23—C28—N8	−0.2 (3)
F38—C44—C45—C46	−179.6 (2)	N7—C23—C28—C27	−179.8 (2)
F39—C45—C46—F40	1.2 (3)	C22—N7—C23—C24	−179.2 (3)
F39—C45—C46—C41	−179.4 (2)	C22—N7—C23—C28	−0.3 (3)
C41—C42—C43—I6	−177.57 (18)	C22—N8—C28—C23	0.7 (3)
C41—C42—C43—C44	1.1 (4)	C22—N8—C28—C27	−179.8 (3)
C42—C41—C46—F40	178.0 (2)	C23—N7—C22—S4	179.87 (19)
C42—C41—C46—C45	−1.3 (4)	C23—N7—C22—N8	0.8 (3)
C42—C43—C44—F38	178.4 (2)	C23—C24—C25—C26	−0.3 (4)
C42—C43—C44—C45	−1.2 (4)	C24—C23—C28—N8	178.7 (2)
C43—C44—C45—F39	−179.2 (2)	C24—C23—C28—C27	−0.8 (4)
C43—C44—C45—C46	0.0 (4)	C24—C25—C26—C27	−0.2 (4)
C44—C45—C46—F40	−178.1 (2)	C25—C26—C27—C28	0.2 (4)
C44—C45—C46—C41	1.3 (4)	C26—C27—C28—N8	−179.1 (3)
C46—C41—C42—F37	179.8 (2)	C26—C27—C28—C23	0.3 (4)
C46—C41—C42—C43	0.1 (4)	C28—N8—C22—S4	179.97 (19)
N1—C2—C3—C4	176.7 (3)	C28—N8—C22—N7	−1.0 (3)
N1—C2—C7—N2	0.4 (3)	C28—C23—C24—C25	0.8 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···S2^{i}	0.85 (2)	2.52 (2)	3.357 (2)	172 (3)
N2—H*N*2···S2	0.85 (2)	2.46 (2)	3.297 (2)	166 (2)
N3—H*N*3···S1	0.85 (2)	2.51 (2)	3.348 (2)	173 (3)
N4—H*N*4···S1^{ii}	0.85 (2)	2.50 (2)	3.326 (2)	166 (2)
N5—H*N*5···S4^{i}	0.85 (2)	2.49 (2)	3.326 (2)	169 (3)
N6—H*N*6···S4	0.85 (2)	2.43 (2)	3.270 (2)	169 (3)
C17—H17···F36^{iii}	0.95	2.61	3.385 (3)	139
C20—H20···F36^{iv}	0.95	2.51	3.235 (3)	133

N7—H*N*7···S3	0.84 (2)	2.47 (2)	3.300 (2)	170 (3)
N8—H*N*8···S3^{ii}	0.85 (2)	2.48 (2)	3.302 (2)	163 (3)

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

1*H*-1,3-Benzodiazole-2-thiol–1,2,4,5-tetrafluoro-3,6-diiodobenzene (1/1) (MBZIM_14F4DIB)

Crystal data

$C_6F_4I_2·C_7H_6N_2S$
M_r = 552.06
Monoclinic, $P2_1/c$
a = 5.5641 (2) Å
b = 33.1320 (11) Å
c = 8.4710 (3) Å
β = 92.754 (1)°
V = 1559.82 (9) Å^3
Z = 4
F(000) = 1024
D_x = 2.351 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 9812 reflections
θ = 2.5–30.2°
μ = 4.20 mm^{-1}
T = 100 K
Plate, colourless
0.22 × 0.18 × 0.06 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec I*μ*S
φ and *ω* scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.501, T_{max} = 0.746
45583 measured reflections
4579 independent reflections
4211 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 30.2°, θ_{min} = 2.5°
h = −7→7
k = −46→46
l = −11→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.044
S = 1.12
4579 reflections
207 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0059P)^2 + 1.8833P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.67 e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.61301 (2)	0.38195 (2)	0.76376 (2)	0.01796 (4)
I2	0.89550 (3)	0.17772 (2)	0.69482 (2)	0.02372 (4)
F1	1.0451 (2)	0.33570 (4)	0.60867 (16)	0.0251 (3)
F2	1.1463 (3)	0.25762 (4)	0.57675 (17)	0.0283 (3)
F3	0.4636 (3)	0.22323 (4)	0.85802 (18)	0.0292 (3)
F4	0.3576 (2)	0.30171 (4)	0.88704 (18)	0.0285 (3)

C8	0.6955 (4)	0.32080 (6)	0.7457 (2)	0.0160 (4)
C9	0.8965 (4)	0.30829 (6)	0.6680 (2)	0.0176 (4)
C10	0.9499 (4)	0.26788 (7)	0.6526 (2)	0.0182 (4)
C11	0.8062 (4)	0.23834 (6)	0.7151 (2)	0.0174 (4)
C12	0.6066 (4)	0.25062 (7)	0.7940 (3)	0.0188 (4)
C13	0.5531 (4)	0.29113 (7)	0.8091 (3)	0.0193 (4)
S1	0.58078 (9)	0.48006 (2)	0.75000 (6)	0.01583 (10)
N1	0.2303 (3)	0.52614 (5)	0.8744 (2)	0.0153 (3)
HN1	0.276 (5)	0.5218 (8)	0.969 (3)	0.023 (7)*
N2	0.2252 (3)	0.52735 (5)	0.6175 (2)	0.0149 (3)
HN2	0.276 (5)	0.5229 (8)	0.525 (3)	0.023 (7)*
C1	0.3405 (4)	0.51181 (6)	0.7471 (2)	0.0143 (4)
C2	0.0446 (4)	0.55224 (6)	0.8266 (2)	0.0147 (4)
C3	−0.1194 (4)	0.57380 (6)	0.9113 (2)	0.0180 (4)
H00G	−0.116250	0.573127	1.023460	0.022*
C4	−0.2889 (4)	0.59651 (7)	0.8238 (3)	0.0196 (4)
H00M	−0.404740	0.611727	0.877214	0.024*
C5	−0.2920 (4)	0.59733 (7)	0.6581 (3)	0.0203 (4)
H00J	−0.409996	0.613183	0.602105	0.024*
C6	−0.1275 (4)	0.57565 (6)	0.5737 (2)	0.0186 (4)
H00L	−0.130222	0.576283	0.461502	0.022*
C7	0.0408 (4)	0.55303 (6)	0.6613 (2)	0.0147 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.02099 (7)	0.01539 (7)	0.01731 (7)	0.00072 (5)	−0.00093 (5)	−0.00014 (5)
I2	0.03021 (8)	0.01541 (7)	0.02536 (8)	0.00224 (6)	−0.00059 (6)	−0.00099 (5)
F1	0.0259 (7)	0.0215 (6)	0.0286 (7)	−0.0048 (6)	0.0099 (6)	0.0039 (5)
F2	0.0264 (7)	0.0260 (7)	0.0339 (8)	0.0022 (6)	0.0152 (6)	−0.0012 (6)
F3	0.0255 (7)	0.0191 (7)	0.0440 (9)	−0.0047 (6)	0.0132 (6)	0.0058 (6)
F4	0.0222 (7)	0.0248 (7)	0.0400 (8)	0.0019 (6)	0.0160 (6)	0.0021 (6)
C8	0.0175 (9)	0.0145 (9)	0.0159 (9)	0.0007 (8)	−0.0011 (7)	−0.0006 (7)
C9	0.0195 (10)	0.0183 (10)	0.0151 (9)	−0.0039 (8)	0.0025 (8)	0.0026 (7)
C10	0.0171 (10)	0.0210 (10)	0.0169 (9)	0.0011 (8)	0.0036 (8)	−0.0004 (8)
C11	0.0199 (10)	0.0146 (9)	0.0174 (10)	−0.0004 (8)	−0.0018 (8)	−0.0009 (7)
C12	0.0187 (10)	0.0178 (10)	0.0200 (10)	−0.0040 (8)	0.0030 (8)	0.0013 (8)
C13	0.0172 (10)	0.0202 (10)	0.0207 (10)	0.0021 (8)	0.0041 (8)	−0.0001 (8)
S1	0.0208 (2)	0.0150 (2)	0.0116 (2)	0.00308 (19)	0.00018 (18)	−0.00025 (16)
N1	0.0177 (8)	0.0184 (8)	0.0096 (8)	0.0020 (7)	−0.0017 (6)	−0.0003 (6)
N2	0.0175 (8)	0.0172 (8)	0.0101 (8)	0.0005 (7)	0.0010 (6)	−0.0007 (6)
C1	0.0180 (9)	0.0129 (9)	0.0119 (8)	−0.0026 (8)	−0.0003 (7)	−0.0004 (7)
C2	0.0150 (9)	0.0152 (9)	0.0139 (9)	−0.0016 (8)	−0.0011 (7)	0.0003 (7)
C3	0.0198 (10)	0.0191 (10)	0.0151 (9)	−0.0017 (8)	0.0010 (8)	−0.0029 (7)
C4	0.0182 (10)	0.0201 (10)	0.0206 (10)	0.0009 (8)	0.0021 (8)	−0.0022 (8)
C5	0.0191 (10)	0.0186 (10)	0.0229 (11)	0.0009 (8)	−0.0017 (8)	0.0021 (8)
C6	0.0203 (10)	0.0212 (10)	0.0139 (9)	0.0000 (8)	−0.0021 (8)	0.0021 (7)
C7	0.0158 (9)	0.0158 (9)	0.0125 (9)	−0.0017 (8)	−0.0006 (7)	−0.0007 (7)

Geometric parameters (Å, º)

I1—C8	2.084 (2)	N1—C2	1.393 (3)
I2—C11	2.078 (2)	N2—HN2	0.86 (3)
F1—C9	1.342 (2)	N2—C1	1.347 (3)
F2—C10	1.338 (2)	N2—C7	1.397 (3)
F3—C12	1.338 (2)	C2—C3	1.385 (3)
F4—C13	1.346 (2)	C2—C7	1.400 (3)
C8—C9	1.388 (3)	C3—H00G	0.9500
C8—C13	1.387 (3)	C3—C4	1.392 (3)
C9—C10	1.379 (3)	C4—H00M	0.9500
C10—C11	1.386 (3)	C4—C5	1.402 (3)
C11—C12	1.384 (3)	C5—H00J	0.9500
C12—C13	1.382 (3)	C5—C6	1.388 (3)
S1—C1	1.700 (2)	C6—H00L	0.9500
N1—HN1	0.84 (3)	C6—C7	1.387 (3)
N1—C1	1.352 (2)		

C9—C8—I1	120.68 (15)	C7—N2—HN2	128.7 (18)
C13—C8—I1	121.91 (15)	N1—C1—S1	126.31 (16)
C13—C8—C9	117.41 (19)	N2—C1—S1	126.27 (15)
F1—C9—C8	120.03 (19)	N2—C1—N1	107.42 (18)
F1—C9—C10	118.85 (18)	N1—C2—C7	106.11 (17)
C10—C9—C8	121.11 (19)	C3—C2—N1	131.90 (19)
F2—C10—C9	118.48 (19)	C3—C2—C7	121.97 (19)
F2—C10—C11	120.25 (19)	C2—C3—H00G	121.6
C9—C10—C11	121.27 (19)	C2—C3—C4	116.70 (19)
C10—C11—I2	120.42 (15)	C4—C3—H00G	121.6
C12—C11—I2	121.65 (16)	C3—C4—H00M	119.4
C12—C11—C10	117.92 (19)	C3—C4—C5	121.2 (2)
F3—C12—C11	120.16 (19)	C5—C4—H00M	119.4
F3—C12—C13	119.09 (19)	C4—C5—H00J	119.0
C13—C12—C11	120.75 (19)	C6—C5—C4	121.9 (2)
F4—C13—C8	119.71 (19)	C6—C5—H00J	119.0
F4—C13—C12	118.75 (19)	C5—C6—H00L	121.7
C12—C13—C8	121.54 (19)	C7—C6—C5	116.65 (19)
C1—N1—HN1	125.0 (18)	C7—C6—H00L	121.7
C1—N1—C2	110.19 (17)	N2—C7—C2	106.19 (17)
C2—N1—HN1	124.6 (18)	C6—C7—N2	132.27 (18)
C1—N2—HN2	121.0 (19)	C6—C7—C2	121.53 (19)
C1—N2—C7	110.07 (17)		

I1—C8—C9—F1	2.5 (3)	C13—C8—C9—F1	−177.88 (19)
I1—C8—C9—C10	−178.66 (16)	C13—C8—C9—C10	1.0 (3)
I1—C8—C13—F4	−1.1 (3)	N1—C2—C3—C4	−178.1 (2)
I1—C8—C13—C12	178.80 (17)	N1—C2—C7—N2	−0.1 (2)
I2—C11—C12—F3	−0.8 (3)	N1—C2—C7—C6	178.62 (19)
I2—C11—C12—C13	178.65 (17)	C1—N1—C2—C3	179.2 (2)

F1—C9—C10—F2	−1.0 (3)	C1—N1—C2—C7	1.0 (2)
F1—C9—C10—C11	178.30 (19)	C1—N2—C7—C2	−0.9 (2)
F2—C10—C11—I2	0.8 (3)	C1—N2—C7—C6	−179.4 (2)
F2—C10—C11—C12	179.3 (2)	C2—N1—C1—S1	178.30 (15)
F3—C12—C13—F4	−0.4 (3)	C2—N1—C1—N2	−1.6 (2)
F3—C12—C13—C8	179.7 (2)	C2—C3—C4—C5	0.0 (3)
C8—C9—C10—F2	−179.86 (19)	C3—C2—C7—N2	−178.50 (19)
C8—C9—C10—C11	−0.6 (3)	C3—C2—C7—C6	0.2 (3)
C9—C8—C13—F4	179.28 (19)	C3—C4—C5—C6	0.1 (3)
C9—C8—C13—C12	−0.8 (3)	C4—C5—C6—C7	0.0 (3)
C9—C10—C11—I2	−178.52 (17)	C5—C6—C7—N2	178.2 (2)
C9—C10—C11—C12	0.0 (3)	C5—C6—C7—C2	−0.1 (3)
C10—C11—C12—F3	−179.3 (2)	C7—N2—C1—S1	−178.36 (15)
C10—C11—C12—C13	0.2 (3)	C7—N2—C1—N1	1.5 (2)
C11—C12—C13—F4	−179.8 (2)	C7—C2—C3—C4	−0.1 (3)
C11—C12—C13—C8	0.3 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···S1^{i}	0.84 (3)	2.47 (3)	3.3089 (18)	172 (2)
N2—H*N*2···S1^{ii}	0.86 (3)	2.50 (3)	3.3527 (17)	172 (2)

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

1*H*-1,3-Benzodiazole-2-thiol–1,1,2,2-tetraiodoethene (1/1) (MBZIM_TIE)

Crystal data

$C_2I_4{\cdot}C_7H_6N_2S$
M_r = 681.82
Orthorhombic, *Pnma*
a = 11.7547 (10) Å
b = 8.3525 (7) Å
c = 15.1077 (13) Å
V = 1483.3 (2) Å^3
Z = 4
F(000) = 1208
D_x = 3.053 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 32859 reflections
θ = 2.2–28.5°
μ = 8.52 mm^{-1}
T = 100 K
Plank, colourless
0.30 × 0.14 × 0.11 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec I*μ*S
φ and *ω* scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.256, T_{max} = 0.746
32859 measured reflections
1993 independent reflections
1885 reflections with $I > 2\sigma(I)$
R_{int} = 0.055
θ_{max} = 28.5°, θ_{min} = 2.2°
h = −15→15
k = −11→11
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.062
S = 1.25
1993 reflections
89 parameters
0 restraints

Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0213P)^2 + 6.7951P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.25$ e Å^{-3}
$\Delta\rho_{min} = -1.48$ e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.71885 (3)	0.250000	0.41396 (2)	0.01158 (9)
I2	0.48169 (3)	0.250000	0.27066 (2)	0.01399 (9)
I3	0.29263 (3)	0.250000	0.46197 (2)	0.01401 (9)
I4	0.52953 (3)	0.250000	0.60280 (2)	0.02001 (10)
C5	0.5414 (5)	0.250000	0.4030 (4)	0.0165 (11)
C6	0.4724 (5)	0.250000	0.4721 (4)	0.0174 (11)
S1	1.01449 (11)	0.250000	0.45747 (8)	0.0100 (2)
N1	0.9064 (3)	0.3808 (4)	0.5997 (2)	0.0103 (6)
HN1	0.925 (4)	0.478 (6)	0.586 (3)	0.016 (12)*
C1	0.9436 (4)	0.250000	0.5556 (3)	0.0113 (10)
C2	0.8394 (3)	0.3332 (4)	0.6716 (2)	0.0101 (7)
C3	0.7765 (3)	0.4217 (5)	0.7322 (2)	0.0124 (7)
H3	0.776830	0.535466	0.732234	0.015*
C4	0.7128 (3)	0.3335 (5)	0.7928 (2)	0.0134 (7)
H4	0.668132	0.388696	0.835332	0.016*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.00779 (16)	0.01634 (17)	0.01059 (16)	0.000	−0.00164 (11)	0.000
I2	0.01027 (17)	0.02331 (19)	0.00839 (16)	0.000	−0.00137 (11)	0.000
I3	0.00843 (16)	0.01822 (18)	0.01538 (17)	0.000	0.00119 (12)	0.000
I4	0.01263 (18)	0.0392 (2)	0.00821 (17)	0.000	−0.00150 (12)	0.000
C5	0.012 (3)	0.023 (3)	0.014 (3)	0.000	−0.002 (2)	0.000
C6	0.019 (3)	0.025 (3)	0.008 (2)	0.000	−0.004 (2)	0.000
S1	0.0102 (5)	0.0095 (5)	0.0102 (5)	0.000	0.0029 (4)	0.000
N1	0.0103 (14)	0.0088 (14)	0.0117 (14)	−0.0008 (11)	0.0015 (11)	−0.0004 (11)
C1	0.008 (2)	0.014 (2)	0.012 (2)	0.000	−0.0048 (18)	0.000
C2	0.0090 (15)	0.0123 (18)	0.0090 (15)	0.0000 (13)	−0.0024 (12)	−0.0001 (13)
C3	0.0132 (17)	0.0116 (16)	0.0125 (16)	0.0013 (13)	0.0002 (13)	−0.0011 (13)
C4	0.0109 (16)	0.0172 (19)	0.0119 (16)	0.0023 (14)	0.0030 (13)	−0.0017 (14)

Geometric parameters (Å, º)

I1—C5	2.093 (6)	N1—C2	1.400 (4)
I2—C5	2.119 (6)	C2—C2^{i}	1.390 (7)
I3—C6	2.118 (6)	C2—C3	1.389 (5)
I4—C6	2.086 (5)	C3—H3	0.9500
C5—C6	1.321 (8)	C3—C4	1.393 (5)
S1—C1	1.701 (6)	C4—C4^{i}	1.395 (8)
N1—HN1	0.87 (5)	C4—H4	0.9500
N1—C1	1.352 (4)		
I1—C5—I2	113.9 (3)	N1^{i}—C1—N1	107.8 (5)
C6—C5—I1	123.3 (4)	C2^{i}—C2—N1	106.5 (2)
C6—C5—I2	122.8 (4)	C3—C2—N1	131.3 (3)
I4—C6—I3	112.9 (3)	C3—C2—C2^{i}	122.2 (2)
C5—C6—I3	123.7 (4)	C2—C3—H3	122.1
C5—C6—I4	123.3 (5)	C2—C3—C4	115.9 (3)
C1—N1—HN1	124 (3)	C4—C3—H3	122.1
C1—N1—C2	109.6 (3)	C3—C4—C4^{i}	121.9 (2)
C2—N1—HN1	127 (3)	C3—C4—H4	119.0
N1—C1—S1	126.0 (2)	C4^{i}—C4—H4	119.0
N1^{i}—C1—S1	126.0 (2)		
I1—C5—C6—I3	180.000 (1)	C1—N1—C2—C3	−174.9 (4)
I1—C5—C6—I4	0.000 (1)	C2—N1—C1—S1	172.5 (3)
I2—C5—C6—I3	0.000 (1)	C2—N1—C1—N1^{i}	−2.6 (5)
I2—C5—C6—I4	180.000 (1)	C2^{i}—C2—C3—C4	−0.3 (4)
N1—C2—C3—C4	175.8 (4)	C2—C3—C4—C4^{i}	0.3 (4)
C1—N1—C2—C2^{i}	1.6 (3)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···S1^{ii}	0.87 (5)	2.47 (5)	3.335 (3)	178 (5)
C3—H3···I1^{iii}	0.95	3.28	3.881 (4)	123

Symmetry codes: (ii) −*x*+2, −*y*+1, −*z*+1; (iii) −*x*+3/2, −*y*+1, *z*+1/2.

5-Methyl-1*H*-1,3-benzodiazole-2-thiol–1,2,3,4-tetrafluoro-5,6-diiodobenzene (1/1) (MMBZIM_12F4DIB)

Crystal data

$C_6F_4I_2·C_8H_8N_2S$
M_r = 566.08
Triclinic, $P\overline{1}$
a = 4.5504 (5) Å
b = 13.2872 (14) Å
c = 13.8064 (14) Å
α = 94.766 (4)°
β = 98.124 (4)°
γ = 99.588 (4)°
V = 809.97 (15) Å^3
Z = 2
F(000) = 528
D_x = 2.321 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 9940 reflections
θ = 2.3–27.5°

μ = 4.05 mm^{-1}
T = 100 K

Needle, colourless
0.19 × 0.07 × 0.04 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec IμS
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.636, T_{max} = 0.746
21426 measured reflections

3704 independent reflections
3174 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 27.5°, θ_{min} = 2.3°
h = −5→5
k = −17→17
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.055
S = 1.24
3704 reflections
217 parameters
1 restraint
Primary atom site location: dual

Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + 2.2494P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.33 e Å^{-3}
$\Delta\rho_{min}$ = −1.06 e Å^{-3}

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.

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

	x	y	z	U_{iso}*/U_{eq}
I1	0.65636 (6)	0.37716 (2)	0.58352 (2)	0.02050 (7)
I2	0.65659 (5)	0.36653 (2)	0.30961 (2)	0.01661 (7)
F1	0.1607 (5)	0.17992 (18)	0.21872 (16)	0.0254 (5)
F2	−0.2407 (6)	0.04739 (19)	0.29154 (19)	0.0334 (6)
F3	−0.2418 (6)	0.05622 (19)	0.4886 (2)	0.0326 (6)
F4	0.1622 (6)	0.1944 (2)	0.61205 (17)	0.0280 (6)
C9	0.3758 (8)	0.2652 (3)	0.4798 (3)	0.0154 (7)
C10	0.3778 (8)	0.2613 (3)	0.3784 (3)	0.0151 (7)
C11	0.1718 (9)	0.1857 (3)	0.3168 (3)	0.0174 (8)
C12	−0.0361 (9)	0.1169 (3)	0.3527 (3)	0.0206 (8)
C13	−0.0373 (9)	0.1222 (3)	0.4535 (3)	0.0206 (8)
C14	0.1684 (9)	0.1943 (3)	0.5145 (3)	0.0182 (8)
S1	−0.0441 (2)	0.50172 (8)	0.83086 (7)	0.0204 (2)
N1	0.2256 (7)	0.3842 (3)	0.9578 (2)	0.0184 (7)
HN1	0.165 (10)	0.414 (4)	1.008 (4)	0.029 (13)*
N2	0.2606 (7)	0.3443 (2)	0.8049 (2)	0.0165 (7)
HN2	0.254 (9)	0.349 (3)	0.7436 (15)	0.009 (10)*
C1	0.1504 (9)	0.4093 (3)	0.8658 (3)	0.0186 (8)
C2	0.3863 (8)	0.3038 (3)	0.9558 (3)	0.0172 (8)

C3	0.5098 (9)	0.2511 (3)	1.0292 (3)	0.0215 (8)
H3	0.493986	0.267954	1.096235	0.026*
C4	0.6580 (9)	0.1726 (3)	1.0008 (3)	0.0222 (8)
H4	0.745045	0.135500	1.049815	0.027*
C5	0.6828 (9)	0.1464 (3)	0.9019 (3)	0.0227 (9)
C6	0.5606 (9)	0.2004 (3)	0.8290 (3)	0.0180 (8)
H6	0.578792	0.184847	0.761942	0.022*
C7	0.4108 (9)	0.2782 (3)	0.8579 (3)	0.0176 (8)
C8	0.8415 (9)	0.0590 (3)	0.8758 (3)	0.0245 (9)
H8A	0.727133	−0.005523	0.890936	0.037*
H8B	1.044903	0.071430	0.914124	0.037*
H8C	0.855211	0.054270	0.805416	0.037*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.02224 (14)	0.02260 (14)	0.01557 (12)	0.00692 (10)	−0.00119 (9)	−0.00285 (10)
I2	0.01925 (13)	0.01578 (12)	0.01588 (12)	0.00435 (9)	0.00466 (9)	0.00245 (9)
F1	0.0295 (13)	0.0253 (13)	0.0173 (11)	−0.0002 (10)	−0.0002 (10)	−0.0036 (10)
F2	0.0269 (14)	0.0274 (14)	0.0386 (15)	−0.0070 (11)	−0.0003 (11)	−0.0060 (11)
F3	0.0246 (13)	0.0283 (14)	0.0489 (17)	0.0016 (11)	0.0171 (12)	0.0143 (12)
F4	0.0320 (14)	0.0389 (15)	0.0181 (12)	0.0110 (11)	0.0106 (10)	0.0116 (11)
C9	0.0157 (18)	0.0167 (18)	0.0136 (17)	0.0051 (15)	0.0014 (14)	−0.0022 (14)
C10	0.0173 (18)	0.0148 (18)	0.0135 (17)	0.0033 (14)	0.0024 (14)	0.0016 (14)
C11	0.0205 (19)	0.0172 (19)	0.0151 (18)	0.0071 (15)	0.0012 (14)	0.0000 (15)
C12	0.0161 (19)	0.0167 (19)	0.027 (2)	0.0010 (15)	0.0000 (15)	−0.0015 (16)
C13	0.0132 (18)	0.0170 (19)	0.035 (2)	0.0052 (15)	0.0101 (16)	0.0061 (17)
C14	0.021 (2)	0.021 (2)	0.0155 (18)	0.0099 (16)	0.0041 (15)	0.0056 (15)
S1	0.0227 (5)	0.0197 (5)	0.0214 (5)	0.0062 (4)	0.0081 (4)	0.0052 (4)
N1	0.0228 (18)	0.0185 (17)	0.0150 (16)	0.0047 (14)	0.0065 (13)	0.0005 (13)
N2	0.0214 (17)	0.0202 (17)	0.0102 (15)	0.0073 (13)	0.0045 (12)	0.0037 (13)
C1	0.021 (2)	0.0172 (19)	0.0179 (19)	−0.0010 (15)	0.0066 (15)	0.0044 (15)
C2	0.0175 (19)	0.0193 (19)	0.0152 (18)	0.0014 (15)	0.0063 (14)	0.0018 (15)
C3	0.024 (2)	0.029 (2)	0.0122 (18)	0.0037 (17)	0.0042 (15)	0.0039 (16)
C4	0.020 (2)	0.026 (2)	0.019 (2)	0.0011 (17)	−0.0010 (15)	0.0054 (16)
C5	0.0158 (19)	0.025 (2)	0.026 (2)	0.0015 (16)	0.0018 (16)	0.0020 (17)
C6	0.0193 (19)	0.0207 (19)	0.0145 (18)	0.0041 (16)	0.0039 (15)	0.0014 (15)
C7	0.0192 (19)	0.0186 (19)	0.0146 (18)	0.0027 (15)	0.0023 (14)	0.0018 (15)
C8	0.020 (2)	0.026 (2)	0.029 (2)	0.0066 (17)	0.0019 (17)	0.0049 (18)

Geometric parameters (Å, º)

I1—C9	2.095 (4)	N2—HN2	0.850 (18)
I2—C10	2.106 (4)	N2—C1	1.358 (5)
F1—C11	1.344 (4)	N2—C7	1.393 (5)
F2—C12	1.340 (4)	C2—C3	1.385 (5)
F3—C13	1.340 (4)	C2—C7	1.391 (5)
F4—C14	1.352 (4)	C3—H3	0.9500

C9—C10	1.399 (5)	C3—C4	1.392 (6)
C9—C14	1.383 (5)	C4—H4	0.9500
C10—C11	1.389 (5)	C4—C5	1.406 (6)
C11—C12	1.377 (6)	C5—C6	1.390 (5)
C12—C13	1.389 (6)	C5—C8	1.511 (6)
C13—C14	1.358 (6)	C6—H6	0.9500
S1—C1	1.693 (4)	C6—C7	1.391 (5)
N1—HN1	0.88 (5)	C8—H8A	0.9800
N1—C1	1.351 (5)	C8—H8B	0.9800
N1—C2	1.392 (5)	C8—H8C	0.9800
C10—C9—I1	123.8 (3)	N2—C1—S1	125.9 (3)
C14—C9—I1	117.3 (3)	C3—C2—N1	132.5 (4)
C14—C9—C10	118.8 (3)	C3—C2—C7	120.7 (4)
C9—C10—I2	125.0 (3)	C7—C2—N1	106.9 (3)
C11—C10—I2	116.6 (3)	C2—C3—H3	121.3
C11—C10—C9	118.3 (4)	C2—C3—C4	117.4 (4)
F1—C11—C10	120.6 (3)	C4—C3—H3	121.3
F1—C11—C12	117.3 (3)	C3—C4—H4	119.0
C12—C11—C10	122.0 (4)	C3—C4—C5	122.1 (4)
F2—C12—C11	120.9 (4)	C5—C4—H4	119.0
F2—C12—C13	120.0 (4)	C4—C5—C8	119.4 (4)
C11—C12—C13	119.1 (4)	C6—C5—C4	120.0 (4)
F3—C13—C12	119.2 (4)	C6—C5—C8	120.6 (4)
F3—C13—C14	121.4 (4)	C5—C6—H6	121.2
C14—C13—C12	119.3 (4)	C5—C6—C7	117.5 (4)
F4—C14—C9	120.6 (3)	C7—C6—H6	121.2
F4—C14—C13	116.9 (4)	C2—C7—N2	105.5 (3)
C13—C14—C9	122.5 (4)	C6—C7—N2	132.2 (3)
C1—N1—HN1	121 (3)	C6—C7—C2	122.3 (3)
C1—N1—C2	110.4 (3)	C5—C8—H8A	109.5
C2—N1—HN1	128 (3)	C5—C8—H8B	109.5
C1—N2—HN2	124 (3)	C5—C8—H8C	109.5
C1—N2—C7	111.0 (3)	H8A—C8—H8B	109.5
C7—N2—HN2	125 (3)	H8A—C8—H8C	109.5
N1—C1—S1	127.9 (3)	H8B—C8—H8C	109.5
N1—C1—N2	106.2 (3)		
I1—C9—C10—I2	−0.5 (5)	C14—C9—C10—C11	−0.4 (5)
I1—C9—C10—C11	−177.4 (3)	N1—C2—C3—C4	179.6 (4)
I1—C9—C14—F4	−3.9 (5)	N1—C2—C7—N2	−0.5 (4)
I1—C9—C14—C13	175.8 (3)	N1—C2—C7—C6	179.7 (4)
I2—C10—C11—F1	1.7 (5)	C1—N1—C2—C3	−179.6 (4)
I2—C10—C11—C12	−175.5 (3)	C1—N1—C2—C7	0.0 (4)
F1—C11—C12—F2	−0.1 (5)	C1—N2—C7—C2	0.8 (4)
F1—C11—C12—C13	−178.3 (3)	C1—N2—C7—C6	−179.4 (4)
F2—C12—C13—F3	1.0 (5)	C2—N1—C1—S1	−180.0 (3)
F2—C12—C13—C14	−178.9 (3)	C2—N1—C1—N2	0.5 (4)

F3—C13—C14—F4	1.7 (5)	C2—C3—C4—C5	−0.2 (6)
F3—C13—C14—C9	−178.0 (3)	C3—C2—C7—N2	179.2 (4)
C9—C10—C11—F1	178.8 (3)	C3—C2—C7—C6	−0.7 (6)
C9—C10—C11—C12	1.5 (6)	C3—C4—C5—C6	0.8 (6)
C10—C9—C14—F4	179.0 (3)	C3—C4—C5—C8	−178.8 (4)
C10—C9—C14—C13	−1.3 (6)	C4—C5—C6—C7	−1.3 (6)
C10—C11—C12—F2	177.2 (3)	C5—C6—C7—N2	−178.5 (4)
C10—C11—C12—C13	−1.0 (6)	C5—C6—C7—C2	1.3 (6)
C11—C12—C13—F3	179.2 (3)	C7—N2—C1—S1	179.6 (3)
C11—C12—C13—C14	−0.7 (6)	C7—N2—C1—N1	−0.8 (4)
C12—C13—C14—F4	−178.4 (3)	C7—C2—C3—C4	0.1 (6)
C12—C13—C14—C9	1.9 (6)	C8—C5—C6—C7	178.3 (4)
C14—C9—C10—I2	176.4 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···S1^{i}	0.88 (5)	2.57 (5)	3.444 (3)	173 (4)
N2—H*N*2···I1	0.85 (2)	3.07 (3)	3.780 (3)	142 (3)
N2—H*N*2···F4	0.85 (2)	2.56 (3)	3.122 (4)	124 (3)
C3—H3···I2^{ii}	0.95	3.06	3.966 (4)	160
C6—H6···F4	0.95	2.63	3.262 (4)	125

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

5-Methyl-1*H*-1,3-benzodiazole-2-thiol–1,2,4,5-tetrafluoro-3,6-diiodobenzene–water (2/1/2) (2MMBZIM_14F4DIB_2H2O)

Crystal data

$C_6F_4I_2·2C_8H_8N_2S·2(H_2O)$
M_r = 766.34
Triclinic, $P\overline{1}$
a = 4.9088 (3) Å
b = 11.4670 (8) Å
c = 11.9686 (8) Å
α = 106.644 (2)°
β = 98.058 (2)°
γ = 92.811 (2)°
V = 636.27 (7) Å^3

Z = 1
F(000) = 370
D_x = 2.000 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 9704 reflections
θ = 3.0–29.6°
μ = 2.69 mm^{-1}
T = 100 K
Plate, colourless
0.31 × 0.11 × 0.08 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec I*μ*S
φ and *ω* scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.536, T_{max} = 0.746
31584 measured reflections

3558 independent reflections
3500 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 29.7°, θ_{min} = 3.0°
h = −6→6
k = −15→15
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.014$
$wR(F^2) = 0.034$
$S = 1.18$
3558 reflections
184 parameters
7 restraints

Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + 0.4884P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.44$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
I1	0.44701 (2)	0.37987 (2)	0.76749 (2)	0.01303 (3)	
F1	0.8875 (2)	0.62085 (8)	0.83664 (8)	0.02138 (19)	
F2	1.31349 (19)	0.70566 (8)	1.01073 (9)	0.02069 (19)	
C9	0.7732 (3)	0.45489 (12)	0.90761 (12)	0.0132 (2)	
C10	0.9374 (3)	0.56045 (13)	0.91719 (13)	0.0143 (3)	
C11	1.1591 (3)	0.60420 (12)	1.00759 (13)	0.0145 (3)	
S1	1.03801 (7)	0.78475 (3)	0.43889 (3)	0.01464 (7)	
N1	0.7347 (3)	0.75457 (11)	0.60568 (11)	0.0147 (2)	
HN1	0.770 (4)	0.6828 (15)	0.5977 (19)	0.023 (5)*	
N2	0.7391 (3)	0.93710 (11)	0.58449 (11)	0.0138 (2)	
HN2	0.788 (4)	1.0008 (16)	0.5627 (18)	0.025 (5)*	
C1	0.8342 (3)	0.82603 (13)	0.54519 (12)	0.0136 (2)	
C2	0.5751 (3)	0.82008 (13)	0.68510 (13)	0.0136 (2)	
C3	0.5789 (3)	0.93718 (12)	0.67155 (12)	0.0129 (2)	
C4	0.4354 (3)	1.02719 (13)	0.73639 (13)	0.0154 (3)	
H4	0.437594	1.106246	0.725878	0.018*	
C5	0.2880 (3)	0.99734 (13)	0.81756 (13)	0.0157 (3)	
C6	0.2857 (3)	0.87925 (14)	0.83004 (13)	0.0173 (3)	
H6	0.183714	0.860585	0.885580	0.021*	
C7	0.4267 (3)	0.78842 (14)	0.76427 (14)	0.0176 (3)	
H7	0.421629	0.708673	0.773170	0.021*	
C8	0.1331 (3)	1.09189 (15)	0.89265 (14)	0.0207 (3)	
H8A	−0.041876	1.052972	0.901230	0.031*	
H8B	0.095344	1.155912	0.854696	0.031*	
H8C	0.245015	1.128188	0.970784	0.031*	
O1	0.7691 (3)	0.49501 (11)	0.54916 (12)	0.0247 (2)	
H1AO	0.936 (5)	0.503 (4)	0.532 (4)	0.023 (10)*	0.5
H1BO	0.594 (5)	0.486 (4)	0.516 (4)	0.034 (13)*	0.5
H2O1	0.778 (6)	0.432 (2)	0.575 (3)	0.063 (9)*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01281 (5)	0.01303 (5)	0.01267 (5)	0.00156 (3)	0.00261 (3)	0.00256 (3)
F1	0.0247 (5)	0.0200 (4)	0.0214 (4)	−0.0027 (4)	−0.0034 (4)	0.0133 (4)
F2	0.0216 (4)	0.0163 (4)	0.0242 (5)	−0.0061 (3)	−0.0011 (4)	0.0096 (4)
C9	0.0124 (6)	0.0130 (6)	0.0129 (6)	0.0018 (5)	0.0027 (5)	0.0016 (5)
C10	0.0160 (6)	0.0138 (6)	0.0145 (6)	0.0027 (5)	0.0034 (5)	0.0058 (5)
C11	0.0152 (6)	0.0114 (6)	0.0171 (6)	0.0000 (5)	0.0044 (5)	0.0037 (5)
S1	0.01389 (15)	0.01446 (15)	0.01405 (15)	0.00125 (12)	0.00305 (12)	0.00144 (12)
N1	0.0158 (6)	0.0114 (5)	0.0165 (6)	0.0028 (4)	0.0036 (5)	0.0031 (4)
N2	0.0140 (5)	0.0117 (5)	0.0161 (6)	0.0008 (4)	0.0037 (4)	0.0039 (4)
C1	0.0117 (6)	0.0133 (6)	0.0136 (6)	0.0005 (5)	−0.0006 (5)	0.0021 (5)
C2	0.0126 (6)	0.0123 (6)	0.0156 (6)	0.0012 (5)	0.0011 (5)	0.0042 (5)
C3	0.0112 (6)	0.0125 (6)	0.0138 (6)	−0.0012 (5)	0.0014 (5)	0.0027 (5)
C4	0.0149 (6)	0.0121 (6)	0.0180 (7)	0.0014 (5)	0.0020 (5)	0.0030 (5)
C5	0.0125 (6)	0.0172 (6)	0.0152 (6)	0.0013 (5)	0.0012 (5)	0.0017 (5)
C6	0.0168 (6)	0.0203 (7)	0.0164 (6)	0.0014 (5)	0.0044 (5)	0.0072 (5)
C7	0.0188 (7)	0.0165 (6)	0.0195 (7)	0.0031 (5)	0.0035 (6)	0.0082 (5)
C8	0.0188 (7)	0.0211 (7)	0.0209 (7)	0.0039 (6)	0.0074 (6)	0.0019 (6)
O1	0.0289 (6)	0.0185 (5)	0.0315 (6)	0.0046 (5)	0.0105 (5)	0.0118 (5)

Geometric parameters (Å, º)

I1—C9	2.0981 (14)	C3—C4	1.3888 (19)
F1—C10	1.3424 (16)	C4—H4	0.9500
F2—C11	1.3452 (16)	C4—C5	1.396 (2)
C9—C10	1.3882 (19)	C5—C6	1.404 (2)
C9—C11^{i}	1.386 (2)	C5—C8	1.509 (2)
C10—C11	1.383 (2)	C6—H6	0.9500
S1—C1	1.7035 (15)	C6—C7	1.392 (2)
N1—HN1	0.830 (15)	C7—H7	0.9500
N1—C1	1.3542 (19)	C8—H8A	0.9800
N1—C2	1.3926 (18)	C8—H8B	0.9800
N2—HN2	0.876 (15)	C8—H8C	0.9800
N2—C1	1.3557 (18)	O1—H1AO	0.880 (18)
N2—C3	1.3905 (18)	O1—H1BO	0.883 (18)
C2—C3	1.3975 (19)	O1—H2O1	0.872 (17)
C2—C7	1.387 (2)		
C10—C9—I1	122.63 (11)	C4—C3—N2	131.65 (13)
C11^{i}—C9—I1	120.13 (10)	C4—C3—C2	121.84 (13)
C11^{i}—C9—C10	117.17 (13)	C3—C4—H4	121.2
F1—C10—C9	120.35 (13)	C3—C4—C5	117.61 (13)
F1—C10—C11	118.48 (12)	C5—C4—H4	121.2
C11—C10—C9	121.15 (13)	C4—C5—C6	119.91 (13)
F2—C11—C9^{i}	120.02 (13)	C4—C5—C8	120.20 (14)
F2—C11—C10	118.29 (13)	C6—C5—C8	119.89 (14)

C10—C11—C9^{i}	121.68 (13)	C5—C6—H6	118.7
C1—N1—HN1	124.2 (15)	C7—C6—C5	122.63 (14)
C1—N1—C2	110.28 (12)	C7—C6—H6	118.7
C2—N1—HN1	125.5 (15)	C2—C7—C6	116.72 (14)
C1—N2—HN2	123.8 (14)	C2—C7—H7	121.6
C1—N2—C3	110.09 (12)	C6—C7—H7	121.6
C3—N2—HN2	125.8 (14)	C5—C8—H8A	109.5
N1—C1—S1	126.80 (11)	C5—C8—H8B	109.5
N1—C1—N2	107.02 (12)	C5—C8—H8C	109.5
N2—C1—S1	126.17 (11)	H8A—C8—H8B	109.5
N1—C2—C3	106.11 (12)	H8A—C8—H8C	109.5
C7—C2—N1	132.60 (13)	H8B—C8—H8C	109.5
C7—C2—C3	121.28 (13)	H1AO—O1—H2O1	101 (3)
N2—C3—C2	106.49 (12)	H1BO—O1—H2O1	101 (3)

I1—C9—C10—F1	1.58 (19)	C1—N2—C3—C4	−178.92 (15)
I1—C9—C10—C11	−176.86 (10)	C2—N1—C1—S1	−179.80 (11)
F1—C10—C11—F2	0.3 (2)	C2—N1—C1—N2	−0.27 (16)
F1—C10—C11—C9^{i}	−178.58 (13)	C2—C3—C4—C5	0.7 (2)
C9—C10—C11—F2	178.75 (13)	C3—N2—C1—S1	179.96 (11)
C9—C10—C11—C9^{i}	−0.1 (2)	C3—N2—C1—N1	0.44 (16)
C11^{i}—C9—C10—F1	178.54 (12)	C3—C2—C7—C6	−0.8 (2)
C11^{i}—C9—C10—C11	0.1 (2)	C3—C4—C5—C6	−0.9 (2)
N1—C2—C3—N2	0.25 (15)	C3—C4—C5—C8	178.66 (13)
N1—C2—C3—C4	178.92 (13)	C4—C5—C6—C7	0.2 (2)
N1—C2—C7—C6	−179.24 (15)	C5—C6—C7—C2	0.6 (2)
N2—C3—C4—C5	179.03 (14)	C7—C2—C3—N2	−178.58 (13)
C1—N1—C2—C3	0.01 (16)	C7—C2—C3—C4	0.1 (2)
C1—N1—C2—C7	178.65 (16)	C8—C5—C6—C7	−179.33 (14)
C1—N2—C3—C2	−0.43 (16)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···O1	0.83 (2)	2.06 (2)	2.8763 (17)	166 (2)
N2—H*N*2···S1^{ii}	0.88 (2)	2.57 (2)	3.4211 (13)	164 (2)
C4—H4···I1^{iii}	0.95	3.03	3.9505 (14)	164
O1—H1*AO*···O1^{iv}	0.88 (2)	1.85 (2)	2.708 (3)	163 (4)
O1—H1*BO*···O1^{v}	0.88 (2)	1.89 (2)	2.759 (3)	167 (4)
O1—H2*O*1···I1	0.87 (2)	3.16 (3)	3.7419 (12)	126 (2)
O1—H2*O*1···S1^{iv}	0.87 (2)	2.65 (2)	3.4251 (13)	149 (3)

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

5-Methyl-1*H*-1,3-benzodiazole-2-thiol–1,3,5-trifluoro-2,4,6-\ triiodobenzene (1/1) (MMBZIM_135F3I3B)

Crystal data

$C_6F_3I_3 \cdot C_8H_8N_2S$
$M_r = 673.98$
Monoclinic, $P2_1/c$
$a = 15.191$ (2) Å
$b = 5.0074$ (7) Å
$c = 22.715$ (3) Å
$\beta = 97.460$ (6)°
$V = 1713.3$ (4) Å^3
$Z = 4$
$F(000) = 1232$
$D_x = 2.613$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9964 reflections
$\theta = 2.4$–$27.5°$
$\mu = 5.62$ mm^{-1}
$T = 100$ K
Needle, colourless
0.26 × 0.04 × 0.04 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec IμS
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
$T_{min} = 0.582$, $T_{max} = 0.746$
23258 measured reflections
3971 independent reflections
3039 reflections with $I > 2\sigma(I)$
$R_{int} = 0.069$
$\theta_{max} = 27.6°$, $\theta_{min} = 2.1°$
$h = -19 \rightarrow 19$
$k = -6 \rightarrow 6$
$l = -29 \rightarrow 29$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.105$
$S = 1.22$
3971 reflections
215 parameters
1 restraint
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + 32.9663P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 2.36$ e Å^{-3}
$\Delta\rho_{min} = -1.89$ e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.83468 (4)	0.73539 (12)	0.22592 (3)	0.02269 (15)
I2	1.12973 (3)	0.55191 (11)	0.42927 (2)	0.01871 (14)
I3	0.78829 (3)	−0.06392 (11)	0.42073 (2)	0.01766 (13)
F1	1.0160 (3)	0.7879 (10)	0.3105 (2)	0.0238 (11)
F2	0.9829 (3)	0.1538 (10)	0.4578 (2)	0.0217 (11)
F3	0.7534 (3)	0.2862 (11)	0.3013 (2)	0.0226 (11)
C9	0.8839 (5)	0.5360 (16)	0.3041 (4)	0.0161 (16)
C10	0.9672 (5)	0.5984 (17)	0.3334 (4)	0.0166 (17)
C11	1.0030 (5)	0.4712 (18)	0.3850 (4)	0.0190 (17)
C12	0.9504 (5)	0.2824 (17)	0.4079 (3)	0.0146 (16)

C13	0.8652 (5)	0.2139 (17)	0.3811 (4)	0.0178 (17)
C14	0.8346 (5)	0.3458 (17)	0.3285 (4)	0.0159 (16)
S1	0.34092 (13)	1.4956 (4)	0.50777 (9)	0.0186 (4)
N1	0.4563 (5)	1.2204 (15)	0.4472 (3)	0.0196 (15)
HN1	0.505 (4)	1.302 (17)	0.460 (4)	0.024*
N2	0.3181 (5)	1.1018 (15)	0.4239 (3)	0.0179 (15)
HN2	0.264 (7)	1.10 (2)	0.427 (4)	0.021*
C1	0.3721 (5)	1.2703 (16)	0.4592 (4)	0.0160 (16)
C2	0.4551 (5)	1.0249 (17)	0.4036 (4)	0.0173 (17)
C3	0.5223 (6)	0.9016 (18)	0.3782 (4)	0.0206 (18)
H3	0.582456	0.952312	0.389046	0.025*
C4	0.5000 (5)	0.7020 (17)	0.3364 (4)	0.0204 (18)
C5	0.4109 (6)	0.6252 (18)	0.3226 (4)	0.0212 (18)
H5	0.396802	0.484620	0.294924	0.025*
C6	0.3427 (6)	0.7456 (17)	0.3477 (4)	0.0187 (17)
H6	0.282540	0.695837	0.336564	0.022*
C7	0.3663 (5)	0.9433 (18)	0.3902 (4)	0.0183 (17)
C8	0.5709 (6)	0.561 (2)	0.3080 (4)	0.027 (2)
H8A	0.588556	0.398157	0.330193	0.041*
H8B	0.622521	0.679184	0.308275	0.041*
H8C	0.547999	0.515407	0.266904	0.041*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.0241 (3)	0.0236 (3)	0.0196 (3)	0.0058 (2)	0.0002 (2)	0.0034 (2)
I2	0.0134 (2)	0.0228 (3)	0.0198 (3)	−0.0017 (2)	0.0018 (2)	−0.0022 (2)
I3	0.0150 (2)	0.0183 (3)	0.0204 (3)	−0.0014 (2)	0.0050 (2)	−0.0012 (2)
F1	0.023 (3)	0.026 (3)	0.024 (3)	−0.008 (2)	0.005 (2)	0.007 (2)
F2	0.017 (2)	0.027 (3)	0.019 (3)	0.000 (2)	−0.001 (2)	0.005 (2)
F3	0.012 (2)	0.031 (3)	0.023 (3)	−0.002 (2)	−0.0043 (19)	0.000 (2)
C9	0.017 (4)	0.014 (4)	0.017 (4)	0.003 (3)	0.002 (3)	−0.003 (3)
C10	0.011 (4)	0.022 (4)	0.018 (4)	0.000 (3)	0.006 (3)	0.000 (3)
C11	0.015 (4)	0.024 (5)	0.017 (4)	0.002 (3)	−0.001 (3)	−0.003 (3)
C12	0.014 (4)	0.020 (4)	0.009 (4)	0.001 (3)	0.001 (3)	−0.005 (3)
C13	0.015 (4)	0.021 (4)	0.017 (4)	0.001 (3)	0.003 (3)	0.003 (3)
C14	0.012 (4)	0.018 (4)	0.017 (4)	0.000 (3)	0.001 (3)	−0.002 (3)
S1	0.0153 (9)	0.0217 (11)	0.0185 (10)	−0.0007 (8)	0.0010 (8)	−0.0038 (8)
N1	0.017 (3)	0.018 (4)	0.024 (4)	−0.002 (3)	0.002 (3)	−0.002 (3)
N2	0.010 (3)	0.021 (4)	0.022 (4)	0.001 (3)	0.001 (3)	−0.003 (3)
C1	0.019 (4)	0.010 (4)	0.019 (4)	0.002 (3)	0.002 (3)	0.003 (3)
C2	0.017 (4)	0.018 (4)	0.017 (4)	−0.003 (3)	0.005 (3)	0.010 (3)
C3	0.016 (4)	0.021 (4)	0.026 (5)	−0.003 (3)	0.008 (3)	0.003 (4)
C4	0.016 (4)	0.018 (4)	0.028 (5)	−0.002 (3)	0.003 (3)	−0.010 (4)
C5	0.020 (4)	0.021 (4)	0.023 (5)	−0.006 (3)	0.005 (3)	0.002 (4)
C6	0.017 (4)	0.019 (4)	0.019 (4)	−0.002 (3)	0.001 (3)	0.000 (3)
C7	0.009 (3)	0.026 (5)	0.020 (4)	0.004 (3)	0.000 (3)	−0.001 (4)
C8	0.021 (4)	0.032 (5)	0.030 (5)	0.005 (4)	0.010 (4)	−0.003 (4)

Geometric parameters (Å, º)

I1—C9	2.089 (8)	N2—HN2	0.84 (10)
I2—C11	2.093 (8)	N2—C1	1.363 (11)
I3—C13	2.094 (8)	N2—C7	1.378 (11)
F1—C10	1.349 (9)	C2—C3	1.382 (12)
F2—C12	1.342 (9)	C2—C7	1.405 (11)
F3—C14	1.340 (9)	C3—H3	0.9500
C9—C10	1.388 (11)	C3—C4	1.390 (12)
C9—C14	1.372 (12)	C4—C5	1.402 (11)
C10—C11	1.381 (12)	C4—C8	1.500 (12)
C11—C12	1.382 (12)	C5—H5	0.9500
C12—C13	1.399 (11)	C5—C6	1.384 (12)
C13—C14	1.391 (11)	C6—H6	0.9500
S1—C1	1.688 (8)	C6—C7	1.396 (12)
N1—HN1	0.86 (2)	C8—H8A	0.9800
N1—C1	1.365 (11)	C8—H8B	0.9800
N1—C2	1.391 (11)	C8—H8C	0.9800
C10—C9—I1	120.3 (6)	N2—C1—N1	106.1 (7)
C14—C9—I1	121.5 (6)	N1—C2—C7	106.4 (7)
C14—C9—C10	118.2 (8)	C3—C2—N1	132.1 (8)
F1—C10—C9	119.0 (7)	C3—C2—C7	121.3 (8)
F1—C10—C11	118.5 (7)	C2—C3—H3	120.7
C11—C10—C9	122.5 (8)	C2—C3—C4	118.7 (8)
C10—C11—I2	123.7 (6)	C4—C3—H3	120.7
C10—C11—C12	116.9 (7)	C3—C4—C5	119.4 (8)
C12—C11—I2	119.5 (6)	C3—C4—C8	120.4 (8)
F2—C12—C11	118.6 (7)	C5—C4—C8	120.1 (8)
F2—C12—C13	117.9 (7)	C4—C5—H5	118.6
C11—C12—C13	123.4 (8)	C6—C5—C4	122.8 (8)
C12—C13—I3	120.8 (6)	C6—C5—H5	118.6
C14—C13—I3	122.8 (6)	C5—C6—H6	121.5
C14—C13—C12	116.4 (8)	C5—C6—C7	117.1 (8)
F3—C14—C9	119.0 (7)	C7—C6—H6	121.5
F3—C14—C13	118.4 (7)	N2—C7—C2	106.1 (7)
C9—C14—C13	122.6 (8)	N2—C7—C6	133.3 (7)
C1—N1—HN1	129 (7)	C6—C7—C2	120.6 (8)
C1—N1—C2	110.2 (7)	C4—C8—H8A	109.5
C2—N1—HN1	120 (7)	C4—C8—H8B	109.5
C1—N2—HN2	118 (7)	C4—C8—H8C	109.5
C1—N2—C7	111.2 (7)	H8A—C8—H8B	109.5
C7—N2—HN2	131 (7)	H8A—C8—H8C	109.5
N1—C1—S1	127.0 (6)	H8B—C8—H8C	109.5
N2—C1—S1	126.9 (6)		
I1—C9—C10—F1	−0.4 (10)	C14—C9—C10—C11	1.9 (13)
I1—C9—C10—C11	−179.5 (6)	N1—C2—C3—C4	177.5 (9)

I1—C9—C14—F3	0.4 (11)	N1—C2—C7—N2	2.9 (9)
I1—C9—C14—C13	−178.8 (6)	N1—C2—C7—C6	−179.7 (8)
I2—C11—C12—F2	−0.8 (10)	C1—N1—C2—C3	−177.6 (9)
I2—C11—C12—C13	−179.5 (6)	C1—N1—C2—C7	−2.6 (9)
I3—C13—C14—F3	−2.0 (11)	C1—N2—C7—C2	−2.3 (10)
I3—C13—C14—C9	177.2 (6)	C1—N2—C7—C6	−179.2 (9)
F1—C10—C11—I2	−0.8 (11)	C2—N1—C1—S1	−178.7 (6)
F1—C10—C11—C12	178.6 (7)	C2—N1—C1—N2	1.2 (9)
F2—C12—C13—I3	3.6 (10)	C2—C3—C4—C5	−2.1 (13)
F2—C12—C13—C14	−178.2 (7)	C2—C3—C4—C8	−179.5 (8)
C9—C10—C11—I2	178.3 (6)	C3—C2—C7—N2	178.5 (8)
C9—C10—C11—C12	−2.3 (13)	C3—C2—C7—C6	−4.0 (13)
C10—C9—C14—F3	179.0 (7)	C3—C4—C5—C6	2.0 (14)
C10—C9—C14—C13	−0.2 (13)	C4—C5—C6—C7	−2.7 (13)
C10—C11—C12—F2	179.8 (7)	C5—C6—C7—N2	−179.7 (9)
C10—C11—C12—C13	1.1 (13)	C5—C6—C7—C2	3.7 (13)
C11—C12—C13—I3	−177.6 (6)	C7—N2—C1—S1	−179.4 (6)
C11—C12—C13—C14	0.5 (12)	C7—N2—C1—N1	0.7 (10)
C12—C13—C14—F3	179.9 (7)	C7—C2—C3—C4	3.1 (13)
C12—C13—C14—C9	−0.9 (12)	C8—C4—C5—C6	179.4 (9)
C14—C9—C10—F1	−179.0 (7)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···S1^{i}	0.86 (2)	2.57 (2)	3.427 (7)	174 (9)
N2—H*N*2···I2^{ii}	0.84 (10)	3.03 (10)	3.657 (7)	133 (8)
C3—H3···I3^{iii}	0.95	3.12	4.035 (9)	163
C6—H6···I1^{iv}	0.95	3.14	3.927 (8)	142

Symmetry codes: (i) −*x*+1, −*y*+3, −*z*+1; (ii) *x*−1, *y*+1, *z*; (iii) *x*, *y*+1, *z*; (iv) −*x*+1, *y*−1/2, −*z*+1/2.

1,3-Benzoxazole-2-thiol–1,2,3,4-tetrafluoro-5,6-diiodobenzene (1/1) (MBZOX_12F4DIB)

Crystal data

$C_6F_4I_2·C_7H_5NOS$
M_r = 553.04
Monoclinic, $P2_1/n$
a = 13.7789 (12) Å
b = 4.4129 (4) Å
c = 25.252 (2) Å
β = 96.337 (3)°
V = 1526.0 (2) Å^3
Z = 4
F(000) = 1024
D_x = 2.407 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 5954 reflections
θ = 3.0–26.8°
μ = 4.30 mm^{-1}
T = 100 K
Needle, colourless
0.46 × 0.06 × 0.02 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec I*μ*S
φ and *ω* scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.578, T_{max} = 0.745
12498 measured reflections
3210 independent reflections

2510 reflections with $I > 2\sigma(I)$
$R_{int} = 0.066$
$\theta_{max} = 26.8°$, $\theta_{min} = 3.0°$
$h = -17 \rightarrow 17$
$k = -5 \rightarrow 5$
$l = -31 \rightarrow 31$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.087$
$S = 1.11$
3210 reflections
203 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0191P)^2 + 7.3427P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.58$ e Å^{-3}
$\Delta\rho_{min} = -1.52$ e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.30796 (3)	−0.08467 (10)	0.67864 (2)	0.02151 (14)
I2	0.44314 (3)	−0.05194 (10)	0.81380 (2)	0.01770 (13)
F1	0.6245 (3)	0.3640 (9)	0.80387 (17)	0.0263 (10)
F2	0.6876 (3)	0.6765 (10)	0.7230 (2)	0.0339 (11)
F3	0.5903 (3)	0.6411 (10)	0.62370 (19)	0.0350 (11)
F4	0.4320 (3)	0.2897 (10)	0.60463 (17)	0.0298 (10)
C8	0.4399 (5)	0.1468 (15)	0.6957 (3)	0.0158 (15)
C9	0.4896 (5)	0.1682 (14)	0.7472 (3)	0.0158 (15)
C10	0.5749 (5)	0.3417 (15)	0.7561 (3)	0.0180 (16)
C11	0.6078 (5)	0.4963 (15)	0.7141 (3)	0.0250 (17)
C12	0.5583 (6)	0.4836 (16)	0.6629 (3)	0.0273 (18)
C13	0.4767 (5)	0.3023 (16)	0.6542 (3)	0.0209 (16)
S1	0.07783 (13)	0.0388 (4)	0.57938 (7)	0.0193 (4)
O1	0.2157 (3)	0.4196 (10)	0.55679 (19)	0.0193 (11)
N1	0.1100 (4)	0.3227 (13)	0.4874 (2)	0.0152 (13)
HN1	0.068 (6)	0.228 (18)	0.466 (3)	0.03 (2)*
C1	0.1325 (5)	0.2629 (14)	0.5389 (3)	0.0147 (14)
C2	0.1772 (5)	0.5252 (15)	0.4695 (3)	0.0158 (14)
C3	0.1868 (5)	0.6569 (16)	0.4216 (3)	0.0219 (16)
H3	0.141810	0.617405	0.391053	0.026*
C4	0.2659 (5)	0.8527 (15)	0.4193 (3)	0.0212 (16)
H4	0.274897	0.948201	0.386523	0.025*
C5	0.3316 (6)	0.9111 (16)	0.4637 (3)	0.0229 (16)
H5	0.384448	1.045851	0.460649	0.028*
C6	0.3218 (5)	0.7761 (15)	0.5130 (3)	0.0193 (16)
H6	0.366596	0.813408	0.543631	0.023*
C7	0.2429 (5)	0.5852 (14)	0.5140 (3)	0.0142 (14)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.0210 (3)	0.0213 (2)	0.0210 (3)	−0.0009 (2)	−0.0034 (2)	−0.0037 (2)
I2	0.0223 (2)	0.0177 (2)	0.0130 (2)	0.0024 (2)	0.00165 (18)	−0.00026 (18)
F1	0.018 (2)	0.031 (2)	0.027 (3)	0.0013 (18)	−0.0068 (18)	−0.0058 (19)
F2	0.021 (2)	0.029 (2)	0.052 (3)	−0.0102 (19)	0.010 (2)	−0.003 (2)
F3	0.043 (3)	0.027 (2)	0.039 (3)	−0.001 (2)	0.020 (2)	0.012 (2)
F4	0.041 (3)	0.032 (2)	0.015 (2)	0.005 (2)	−0.001 (2)	0.0042 (19)
C8	0.011 (3)	0.021 (3)	0.016 (4)	0.005 (3)	0.004 (3)	−0.003 (3)
C9	0.016 (3)	0.013 (3)	0.020 (4)	0.005 (3)	0.007 (3)	0.002 (3)
C10	0.016 (4)	0.015 (3)	0.023 (4)	0.004 (3)	−0.001 (3)	−0.006 (3)
C11	0.024 (4)	0.014 (4)	0.038 (5)	0.002 (3)	0.010 (4)	−0.002 (3)
C12	0.037 (5)	0.021 (4)	0.027 (4)	0.005 (3)	0.019 (4)	0.013 (3)
C13	0.027 (4)	0.020 (3)	0.016 (4)	0.010 (3)	0.001 (3)	0.006 (3)
S1	0.0249 (9)	0.0194 (9)	0.0132 (9)	−0.0053 (7)	0.0007 (7)	0.0000 (7)
O1	0.023 (3)	0.017 (2)	0.017 (3)	0.000 (2)	−0.003 (2)	0.003 (2)
N1	0.021 (3)	0.013 (3)	0.010 (3)	0.000 (2)	−0.002 (3)	−0.003 (2)
C1	0.013 (3)	0.012 (3)	0.019 (4)	0.004 (3)	0.003 (3)	−0.002 (3)
C2	0.021 (4)	0.016 (3)	0.011 (4)	0.000 (3)	0.004 (3)	−0.002 (3)
C3	0.026 (4)	0.021 (4)	0.018 (4)	0.000 (3)	0.000 (3)	−0.009 (3)
C4	0.029 (4)	0.016 (3)	0.019 (4)	0.002 (3)	0.005 (3)	0.004 (3)
C5	0.029 (4)	0.018 (4)	0.022 (4)	0.000 (3)	0.008 (3)	0.008 (3)
C6	0.017 (4)	0.018 (4)	0.021 (4)	−0.002 (3)	−0.003 (3)	−0.003 (3)
C7	0.022 (4)	0.012 (3)	0.010 (3)	−0.003 (3)	0.005 (3)	−0.002 (3)

Geometric parameters (Å, º)

I1—C8	2.088 (7)	O1—C7	1.390 (8)
I2—C9	2.101 (7)	N1—HN1	0.85 (8)
F1—C10	1.322 (8)	N1—C1	1.330 (9)
F2—C11	1.355 (8)	N1—C2	1.396 (9)
F3—C12	1.323 (8)	C2—C3	1.364 (10)
F4—C13	1.333 (8)	C2—C7	1.387 (9)
C8—C9	1.406 (10)	C3—H3	0.9500
C8—C13	1.394 (10)	C3—C4	1.397 (10)
C9—C10	1.400 (9)	C4—H4	0.9500
C10—C11	1.380 (11)	C4—C5	1.385 (10)
C11—C12	1.396 (11)	C5—H5	0.9500
C12—C13	1.378 (11)	C5—C6	1.399 (10)
S1—C1	1.662 (7)	C6—H6	0.9500
O1—C1	1.372 (8)	C6—C7	1.378 (9)
C9—C8—I1	123.2 (5)	O1—C1—S1	121.1 (5)
C13—C8—I1	117.8 (5)	N1—C1—S1	130.3 (5)
C13—C8—C9	118.9 (6)	N1—C1—O1	108.6 (6)
C8—C9—I2	123.3 (5)	C3—C2—N1	133.8 (6)
C10—C9—I2	116.7 (5)	C3—C2—C7	121.2 (6)

C10—C9—C8	120.0 (6)	C7—C2—N1	104.9 (6)
F1—C10—C9	121.8 (7)	C2—C3—H3	121.6
F1—C10—C11	118.9 (6)	C2—C3—C4	116.9 (6)
C11—C10—C9	119.3 (7)	C4—C3—H3	121.6
F2—C11—C10	119.5 (7)	C3—C4—H4	119.1
F2—C11—C12	118.9 (7)	C5—C4—C3	121.7 (7)
C10—C11—C12	121.6 (7)	C5—C4—H4	119.1
F3—C12—C11	120.2 (7)	C4—C5—H5	119.3
F3—C12—C13	121.2 (7)	C4—C5—C6	121.4 (7)
C13—C12—C11	118.6 (7)	C6—C5—H5	119.3
F4—C13—C8	121.1 (6)	C5—C6—H6	122.2
F4—C13—C12	117.3 (7)	C7—C6—C5	115.5 (6)
C12—C13—C8	121.5 (7)	C7—C6—H6	122.2
C1—O1—C7	107.2 (5)	C2—C7—O1	108.7 (5)
C1—N1—HN1	126 (6)	C6—C7—O1	128.1 (6)
C1—N1—C2	110.5 (6)	C6—C7—C2	123.2 (6)
C2—N1—HN1	123 (6)		

I1—C8—C9—I2	4.0 (8)	C13—C8—C9—I2	179.9 (5)
I1—C8—C9—C10	−176.3 (5)	C13—C8—C9—C10	−0.5 (10)
I1—C8—C13—F4	−3.7 (9)	N1—C2—C3—C4	−179.9 (7)
I1—C8—C13—C12	173.9 (5)	N1—C2—C7—O1	0.7 (7)
I2—C9—C10—F1	0.7 (8)	N1—C2—C7—C6	179.5 (6)
I2—C9—C10—C11	−178.7 (5)	C1—O1—C7—C2	−1.1 (7)
F1—C10—C11—F2	−2.7 (10)	C1—O1—C7—C6	−180.0 (7)
F1—C10—C11—C12	−179.5 (6)	C1—N1—C2—C3	−179.7 (7)
F2—C11—C12—F3	1.3 (10)	C1—N1—C2—C7	0.1 (7)
F2—C11—C12—C13	−179.3 (6)	C2—N1—C1—S1	−179.8 (5)
F3—C12—C13—F4	0.7 (10)	C2—N1—C1—O1	−0.8 (7)
F3—C12—C13—C8	−177.0 (6)	C2—C3—C4—C5	−0.1 (10)
C8—C9—C10—F1	−179.0 (6)	C3—C2—C7—O1	−179.6 (6)
C8—C9—C10—C11	1.6 (10)	C3—C2—C7—C6	−0.7 (11)
C9—C8—C13—F4	−179.8 (6)	C3—C4—C5—C6	0.1 (11)
C9—C8—C13—C12	−2.2 (10)	C4—C5—C6—C7	−0.4 (10)
C9—C10—C11—F2	176.7 (6)	C5—C6—C7—O1	179.3 (6)
C9—C10—C11—C12	−0.1 (10)	C5—C6—C7—C2	0.7 (10)
C10—C11—C12—F3	178.1 (6)	C7—O1—C1—S1	−179.7 (5)
C10—C11—C12—C13	−2.5 (11)	C7—O1—C1—N1	1.2 (7)
C11—C12—C13—F4	−178.7 (6)	C7—C2—C3—C4	0.3 (10)
C11—C12—C13—C8	3.7 (11)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···S1^{i}	0.85 (8)	2.50 (8)	3.335 (6)	167 (8)
C3—H3···I2^{ii}	0.95	3.19	4.108 (7)	162

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

1,3-Benzoxazole-2-thiol–1,2,3,5-tetrafluoro-4,6-diiodobenzene (1/1) (MBZOX_13F4DIB)

Crystal data

$C_6F_4I_2·C_7H_5NOS$
M_r = 553.04
Monoclinic, $P2_1/c$
a = 15.1655 (8) Å
b = 4.3803 (2) Å
c = 23.0358 (12) Å
β = 99.923 (2)°
V = 1507.36 (13) Å^3
Z = 4
$F(000)$ = 1024
D_x = 2.437 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9330 reflections
θ = 2.7–30.6°
μ = 4.35 mm^{-1}
T = 100 K
Needle, colourless
0.23 × 0.12 × 0.09 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec IμS
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.541, T_{max} = 0.746
39610 measured reflections
4625 independent reflections
4119 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 30.6°, θ_{min} = 2.1°
h = −21→21
k = −6→6
l = −32→32

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.048
S = 1.16
4625 reflections
203 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0088P)^2 + 2.2764P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.96 e Å^{-3}
$\Delta\rho_{min}$ = −1.35 e Å^{-3}

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.

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

	x	y	z	U_{iso}*/U_{eq}
I1	0.71955 (2)	−0.00881 (3)	0.06483 (2)	0.01983 (4)
I2	0.36910 (2)	0.55990 (4)	0.09449 (2)	0.02789 (5)
F1	0.51550 (9)	0.1796 (3)	0.04571 (6)	0.0245 (3)
F2	0.50261 (12)	0.8071 (4)	0.20979 (7)	0.0336 (4)
F3	0.67787 (12)	0.7060 (4)	0.24932 (7)	0.0422 (4)
F4	0.77333 (10)	0.3490 (4)	0.18773 (7)	0.0352 (4)
C8	0.64548 (14)	0.2498 (5)	0.11554 (10)	0.0173 (4)
C9	0.55516 (14)	0.3056 (5)	0.09648 (10)	0.0171 (4)
C10	0.50419 (15)	0.4888 (5)	0.12703 (10)	0.0187 (4)
C11	0.54714 (17)	0.6213 (5)	0.17885 (11)	0.0223 (5)

C12	0.63676 (18)	0.5704 (6)	0.19943 (10)	0.0250 (5)
C13	0.68526 (16)	0.3866 (6)	0.16770 (11)	0.0226 (5)
S1	0.85453 (4)	0.94524 (12)	0.49409 (2)	0.01660 (10)
O1	0.82568 (10)	0.5576 (3)	0.40484 (7)	0.0155 (3)
N1	0.96873 (12)	0.6582 (4)	0.43253 (8)	0.0150 (3)
HN1	1.0171 (19)	0.742 (7)	0.4529 (13)	0.024 (7)*
C1	0.88629 (14)	0.7182 (5)	0.44345 (9)	0.0151 (4)
C2	0.96367 (14)	0.4504 (5)	0.38611 (9)	0.0140 (4)
C3	1.02660 (14)	0.3138 (5)	0.35766 (10)	0.0173 (4)
H3	1.088760	0.354870	0.368581	0.021*
C4	0.99394 (15)	0.1129 (5)	0.31216 (10)	0.0176 (4)
H4	1.035003	0.013545	0.291629	0.021*
C5	0.90240 (15)	0.0533 (5)	0.29583 (10)	0.0182 (4)
H5	0.882849	−0.085313	0.264531	0.022*
C6	0.83913 (14)	0.1930 (5)	0.32450 (10)	0.0177 (4)
H6	0.776786	0.154860	0.313733	0.021*
C7	0.87317 (14)	0.3897 (5)	0.36943 (9)	0.0141 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01738 (7)	0.02028 (7)	0.02311 (8)	0.00339 (5)	0.00709 (5)	0.00604 (5)
I2	0.01897 (8)	0.03084 (9)	0.03563 (10)	0.00756 (6)	0.00974 (6)	0.00672 (7)
F1	0.0175 (6)	0.0307 (8)	0.0242 (7)	−0.0014 (5)	0.0005 (5)	−0.0107 (6)
F2	0.0534 (10)	0.0242 (8)	0.0266 (8)	0.0077 (7)	0.0170 (7)	−0.0037 (6)
F3	0.0559 (11)	0.0436 (10)	0.0218 (8)	−0.0054 (8)	−0.0080 (7)	−0.0099 (7)
F4	0.0236 (7)	0.0491 (10)	0.0282 (8)	0.0008 (7)	−0.0088 (6)	0.0030 (7)
C8	0.0163 (9)	0.0162 (10)	0.0195 (11)	0.0003 (8)	0.0035 (8)	0.0023 (8)
C9	0.0185 (10)	0.0153 (9)	0.0174 (10)	−0.0022 (8)	0.0031 (8)	0.0011 (8)
C10	0.0191 (10)	0.0166 (10)	0.0217 (11)	0.0012 (8)	0.0069 (8)	0.0039 (8)
C11	0.0341 (13)	0.0159 (10)	0.0188 (11)	0.0031 (9)	0.0098 (9)	0.0012 (8)
C12	0.0371 (14)	0.0225 (11)	0.0132 (10)	−0.0046 (10)	−0.0017 (9)	−0.0004 (9)
C13	0.0211 (11)	0.0260 (12)	0.0188 (11)	−0.0016 (9)	−0.0023 (9)	0.0068 (9)
S1	0.0159 (2)	0.0171 (2)	0.0175 (2)	−0.00208 (18)	0.00487 (19)	−0.00332 (19)
O1	0.0127 (7)	0.0170 (7)	0.0166 (7)	−0.0007 (5)	0.0023 (6)	−0.0018 (6)
N1	0.0138 (8)	0.0160 (8)	0.0150 (9)	−0.0025 (6)	0.0022 (6)	−0.0024 (7)
C1	0.0147 (9)	0.0138 (9)	0.0159 (10)	−0.0011 (7)	0.0005 (7)	0.0027 (7)
C2	0.0148 (9)	0.0123 (9)	0.0144 (9)	−0.0004 (7)	0.0015 (7)	0.0013 (7)
C3	0.0149 (9)	0.0189 (10)	0.0184 (10)	0.0007 (8)	0.0037 (8)	0.0027 (8)
C4	0.0205 (10)	0.0166 (10)	0.0166 (10)	0.0019 (8)	0.0059 (8)	0.0020 (8)
C5	0.0228 (10)	0.0173 (10)	0.0147 (10)	−0.0019 (8)	0.0034 (8)	0.0000 (8)
C6	0.0153 (9)	0.0180 (10)	0.0187 (11)	−0.0032 (8)	−0.0005 (8)	−0.0010 (8)
C7	0.0151 (9)	0.0144 (9)	0.0134 (9)	0.0007 (7)	0.0038 (7)	0.0016 (7)

Geometric parameters (Å, º)

I1—C8	2.089 (2)	O1—C7	1.389 (3)
I2—C10	2.080 (2)	N1—HN1	0.88 (3)

F1—C9	1.339 (3)	N1—C1	1.343 (3)
F2—C11	1.339 (3)	N1—C2	1.396 (3)
F3—C12	1.347 (3)	C2—C3	1.383 (3)
F4—C13	1.346 (3)	C2—C7	1.386 (3)
C8—C9	1.386 (3)	C3—H3	0.9500
C8—C13	1.384 (3)	C3—C4	1.393 (3)
C9—C10	1.387 (3)	C4—H4	0.9500
C10—C11	1.385 (3)	C4—C5	1.399 (3)
C11—C12	1.378 (4)	C5—H5	0.9500
C12—C13	1.382 (4)	C5—C6	1.396 (3)
S1—C1	1.666 (2)	C6—H6	0.9500
O1—C1	1.360 (2)	C6—C7	1.377 (3)

C9—C8—I1	121.04 (17)	O1—C1—S1	121.49 (15)
C13—C8—I1	121.61 (17)	N1—C1—S1	129.70 (17)
C13—C8—C9	117.2 (2)	N1—C1—O1	108.82 (18)
F1—C9—C8	118.4 (2)	C3—C2—N1	133.9 (2)
F1—C9—C10	118.4 (2)	C3—C2—C7	121.1 (2)
C8—C9—C10	123.2 (2)	C7—C2—N1	104.99 (18)
C9—C10—I2	120.27 (17)	C2—C3—H3	121.8
C11—C10—I2	122.39 (17)	C2—C3—C4	116.4 (2)
C11—C10—C9	117.3 (2)	C4—C3—H3	121.8
F2—C11—C10	120.5 (2)	C3—C4—H4	119.1
F2—C11—C12	118.2 (2)	C3—C4—C5	121.9 (2)
C12—C11—C10	121.2 (2)	C5—C4—H4	119.1
F3—C12—C11	120.4 (2)	C4—C5—H5	119.3
F3—C12—C13	119.9 (2)	C6—C5—C4	121.5 (2)
C11—C12—C13	119.7 (2)	C6—C5—H5	119.3
F4—C13—C8	120.2 (2)	C5—C6—H6	122.2
F4—C13—C12	118.5 (2)	C7—C6—C5	115.5 (2)
C12—C13—C8	121.3 (2)	C7—C6—H6	122.2
C1—O1—C7	107.32 (16)	C2—C7—O1	108.94 (18)
C1—N1—HN1	122.5 (19)	C6—C7—O1	127.43 (19)
C1—N1—C2	109.92 (18)	C6—C7—C2	123.6 (2)
C2—N1—HN1	127.6 (19)		

I1—C8—C9—F1	2.6 (3)	C13—C8—C9—F1	179.0 (2)
I1—C8—C9—C10	−176.56 (17)	C13—C8—C9—C10	−0.1 (3)
I1—C8—C13—F4	−1.6 (3)	N1—C2—C3—C4	179.9 (2)
I1—C8—C13—C12	176.58 (18)	N1—C2—C7—O1	0.2 (2)
I2—C10—C11—F2	−1.1 (3)	N1—C2—C7—C6	−180.0 (2)
I2—C10—C11—C12	180.00 (18)	C1—O1—C7—C2	−0.6 (2)
F1—C9—C10—I2	0.6 (3)	C1—O1—C7—C6	179.6 (2)
F1—C9—C10—C11	−178.8 (2)	C1—N1—C2—C3	−179.9 (2)
F2—C11—C12—F3	−0.2 (3)	C1—N1—C2—C7	0.3 (2)
F2—C11—C12—C13	−178.2 (2)	C2—N1—C1—S1	179.30 (17)
F3—C12—C13—F4	−0.3 (4)	C2—N1—C1—O1	−0.7 (2)
F3—C12—C13—C8	−178.4 (2)	C2—C3—C4—C5	0.3 (3)

C8—C9—C10—I2	179.72 (17)	C3—C2—C7—O1	−179.62 (19)
C8—C9—C10—C11	0.3 (3)	C3—C2—C7—C6	0.2 (3)
C9—C8—C13—F4	−178.0 (2)	C3—C4—C5—C6	0.0 (3)
C9—C8—C13—C12	0.1 (3)	C4—C5—C6—C7	−0.2 (3)
C9—C10—C11—F2	178.3 (2)	C5—C6—C7—O1	179.9 (2)
C9—C10—C11—C12	−0.6 (3)	C5—C6—C7—C2	0.1 (3)
C10—C11—C12—F3	178.7 (2)	C7—O1—C1—S1	−179.20 (15)
C10—C11—C12—C13	0.7 (4)	C7—O1—C1—N1	0.8 (2)
C11—C12—C13—F4	177.8 (2)	C7—C2—C3—C4	−0.4 (3)
C11—C12—C13—C8	−0.4 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···S1^{i}	0.88 (3)	2.52 (3)	3.3906 (19)	172 (3)
C3—H3···I1^{ii}	0.95	3.10	4.030 (2)	166

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

1,3-Benzoxazole-2-thiol–1,2,4,5-tetrafluoro-3,6-diiodobenzene (2/1) (2MBZOX_14F4DIB)

Crystal data

$C_6F_4I_2·2C_7H_5NOS$
M_r = 704.22
Monoclinic, *C*2/*c*
a = 31.025 (4) Å
b = 4.3159 (5) Å
c = 19.061 (2) Å
β = 114.434 (4)°
V = 2323.6 (5) Å^3
Z = 4
F(000) = 1336
D_x = 2.013 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 9971 reflections
θ = 2.4–28.7°
μ = 2.94 mm^{-1}
T = 100 K
Tabular, colourless
0.29 × 0.12 × 0.03 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec I*μ*S
φ and *ω* scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.637, T_{max} = 0.746
25197 measured reflections
2950 independent reflections
2571 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 28.7°, θ_{min} = 2.2°
h = −41→41
k = −5→5
l = −25→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.060
S = 1.32
2950 reflections
149 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + 11.7646P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 1.54 e Å^{-3}
$\Delta\rho_{min}$ = −1.15 e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.64136 (2)	0.39079 (5)	0.46092 (2)	0.01937 (7)
F1	0.71102 (7)	0.7954 (5)	0.60381 (11)	0.0276 (5)
F2	0.70741 (7)	0.4164 (5)	0.36823 (11)	0.0273 (5)
C8	0.70659 (11)	0.6029 (8)	0.48500 (19)	0.0189 (6)
C9	0.72975 (11)	0.7707 (8)	0.55172 (19)	0.0194 (7)
C10	0.72770 (12)	0.5825 (8)	0.43364 (19)	0.0201 (7)
S1	0.54594 (3)	0.0194 (2)	0.43700 (5)	0.01964 (17)
O1	0.49241 (8)	0.4059 (5)	0.32770 (12)	0.0181 (5)
N1	0.46292 (10)	0.3062 (7)	0.41195 (16)	0.0180 (6)
HN1	0.4609 (14)	0.224 (10)	0.452 (2)	0.028 (11)*
C1	0.49912 (12)	0.2491 (8)	0.39283 (18)	0.0182 (6)
C2	0.43102 (12)	0.5092 (8)	0.35848 (18)	0.0187 (6)
C3	0.38827 (12)	0.6362 (8)	0.35038 (19)	0.0227 (7)
H3	0.374567	0.592471	0.385578	0.027*
C4	0.36660 (12)	0.8320 (8)	0.2875 (2)	0.0253 (7)
H4	0.337264	0.925746	0.279739	0.030*
C5	0.38649 (13)	0.8950 (8)	0.2355 (2)	0.0251 (7)
H5	0.370406	1.030939	0.193581	0.030*
C6	0.42930 (12)	0.7643 (8)	0.24340 (19)	0.0224 (7)
H6	0.443055	0.805267	0.208135	0.027*
C7	0.45026 (11)	0.5714 (7)	0.30592 (18)	0.0181 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01700 (11)	0.01887 (11)	0.02288 (11)	−0.00041 (8)	0.00889 (8)	0.00070 (8)
F1	0.0248 (10)	0.0379 (12)	0.0253 (10)	−0.0054 (9)	0.0154 (9)	−0.0045 (9)
F2	0.0246 (10)	0.0342 (12)	0.0238 (10)	−0.0064 (9)	0.0107 (9)	−0.0095 (9)
C8	0.0180 (15)	0.0161 (15)	0.0231 (16)	−0.0009 (12)	0.0092 (13)	0.0014 (13)
C9	0.0178 (15)	0.0229 (17)	0.0198 (16)	0.0016 (13)	0.0101 (13)	0.0002 (13)
C10	0.0196 (16)	0.0197 (16)	0.0190 (15)	0.0010 (13)	0.0061 (13)	−0.0027 (13)
S1	0.0185 (4)	0.0201 (4)	0.0209 (4)	−0.0009 (3)	0.0089 (3)	0.0015 (3)
O1	0.0198 (11)	0.0198 (12)	0.0159 (10)	−0.0014 (9)	0.0087 (9)	0.0002 (9)
N1	0.0202 (14)	0.0190 (14)	0.0166 (13)	0.0002 (11)	0.0092 (11)	0.0030 (11)
C1	0.0217 (16)	0.0163 (16)	0.0172 (15)	−0.0055 (13)	0.0085 (13)	−0.0038 (12)
C2	0.0239 (17)	0.0140 (15)	0.0164 (15)	−0.0035 (13)	0.0064 (13)	−0.0009 (12)
C3	0.0219 (16)	0.0246 (18)	0.0220 (16)	0.0004 (14)	0.0094 (14)	−0.0018 (14)
C4	0.0212 (17)	0.0241 (19)	0.0289 (18)	−0.0004 (14)	0.0088 (15)	−0.0016 (15)
C5	0.0274 (18)	0.0215 (17)	0.0206 (16)	−0.0003 (15)	0.0041 (14)	0.0016 (14)

C6	0.0274 (18)	0.0226 (18)	0.0174 (16)	−0.0048 (14)	0.0097 (14)	0.0001 (13)
C7	0.0185 (15)	0.0158 (16)	0.0194 (15)	−0.0034 (12)	0.0073 (13)	−0.0026 (12)

Geometric parameters (Å, º)

I1—C8	2.092 (3)	N1—C2	1.397 (4)
F1—C9	1.346 (4)	C2—C3	1.383 (5)
F2—C10	1.347 (4)	C2—C7	1.388 (4)
C8—C9	1.379 (5)	C3—H3	0.9500
C8—C10	1.388 (4)	C3—C4	1.391 (5)
C9—C10^{i}	1.385 (5)	C4—H4	0.9500
S1—C1	1.670 (3)	C4—C5	1.393 (5)
O1—C1	1.352 (4)	C5—H5	0.9500
O1—C7	1.394 (4)	C5—C6	1.393 (5)
N1—HN1	0.87 (4)	C6—H6	0.9500
N1—C1	1.339 (4)	C6—C7	1.376 (5)
C9—C8—I1	121.3 (2)	C3—C2—C7	121.4 (3)
C9—C8—C10	117.8 (3)	C7—C2—N1	105.2 (3)
C10—C8—I1	120.9 (2)	C2—C3—H3	122.1
F1—C9—C8	120.2 (3)	C2—C3—C4	115.9 (3)
F1—C9—C10^{i}	118.8 (3)	C4—C3—H3	122.1
C8—C9—C10^{i}	121.1 (3)	C3—C4—H4	118.9
F2—C10—C8	120.7 (3)	C3—C4—C5	122.2 (3)
F2—C10—C9^{i}	118.1 (3)	C5—C4—H4	118.9
C9^{i}—C10—C8	121.2 (3)	C4—C5—H5	119.1
C1—O1—C7	107.4 (2)	C6—C5—C4	121.8 (3)
C1—N1—HN1	123 (3)	C6—C5—H5	119.1
C1—N1—C2	109.7 (3)	C5—C6—H6	122.4
C2—N1—HN1	128 (3)	C7—C6—C5	115.2 (3)
O1—C1—S1	122.1 (2)	C7—C6—H6	122.4
N1—C1—S1	128.6 (3)	C2—C7—O1	108.5 (3)
N1—C1—O1	109.2 (3)	C6—C7—O1	128.1 (3)
C3—C2—N1	133.4 (3)	C6—C7—C2	123.5 (3)
I1—C8—C9—F1	1.5 (4)	C1—N1—C2—C7	−0.1 (4)
I1—C8—C9—C10^{i}	−178.3 (3)	C2—N1—C1—S1	−179.1 (3)
I1—C8—C10—F2	−2.3 (4)	C2—N1—C1—O1	−0.4 (4)
I1—C8—C10—C9^{i}	178.3 (3)	C2—C3—C4—C5	0.4 (5)
C9—C8—C10—F2	178.5 (3)	C3—C2—C7—O1	−178.4 (3)
C9—C8—C10—C9^{i}	−0.9 (6)	C3—C2—C7—C6	1.1 (5)
C10—C8—C9—F1	−179.4 (3)	C3—C4—C5—C6	0.3 (6)
C10—C8—C9—C10^{i}	0.9 (6)	C4—C5—C6—C7	−0.3 (5)
N1—C2—C3—C4	−179.6 (3)	C5—C6—C7—O1	179.0 (3)
N1—C2—C7—O1	0.5 (3)	C5—C6—C7—C2	−0.4 (5)
N1—C2—C7—C6	180.0 (3)	C7—O1—C1—S1	179.5 (2)
C1—O1—C7—C2	−0.8 (3)	C7—O1—C1—N1	0.8 (3)

C1—O1—C7—C6	179.8 (3)	C7—C2—C3—C4	−1.0 (5)
C1—N1—C2—C3	178.6 (4)		

Symmetry code: (i) −*x*+3/2, −*y*+3/2, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···S1^{ii}	0.87 (4)	2.45 (4)	3.316 (3)	178 (4)
C3—H3···I1^{iii}	0.95	3.16	4.066 (3)	159

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

1,3-Benzoxazole-2-thiol–1,3,5-trifluoro-2,4,6-triiodobenzene (1/1) (MBZOX_135F3I3B)

Crystal data

$C_6F_3I_3·C_7H_5NOS$
M_r = 660.94
Monoclinic, $P2_1/c$
a = 14.9295 (7) Å
b = 4.6119 (2) Å
c = 23.5065 (12) Å
β = 92.548 (2)°
V = 1616.90 (13) Å^3
Z = 4
$F(000)$ = 1200
D_x = 2.715 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9982 reflections
θ = 2.7–26.5°
μ = 5.96 mm^{-1}
T = 100 K
Column, colourless
0.22 × 0.06 × 0.05 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec IμS
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.551, T_{max} = 0.745
19413 measured reflections
3348 independent reflections
2845 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 26.6°, θ_{min} = 2.2°
h = −18→18
k = −5→5
l = −29→29

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.061
S = 1.22
3348 reflections
203 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0015P)^2 + 8.0148P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.80 e Å^{-3}
$\Delta\rho_{min}$ = −0.77 e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.70807 (2)	0.45232 (7)	0.55419 (2)	0.01748 (9)
I2	0.67869 (2)	1.23515 (8)	0.76030 (2)	0.02173 (10)
I3	0.36351 (2)	1.08539 (8)	0.59175 (2)	0.02080 (10)
F1	0.75694 (18)	0.8001 (7)	0.66897 (14)	0.0224 (7)
F2	0.4884 (2)	1.2983 (7)	0.69902 (14)	0.0233 (7)
F3	0.50893 (19)	0.6840 (7)	0.54104 (13)	0.0216 (7)
C8	0.6336 (3)	0.7273 (11)	0.6051 (2)	0.0148 (10)
C9	0.6700 (3)	0.8566 (12)	0.6536 (2)	0.0171 (11)
C10	0.6230 (3)	1.0473 (12)	0.6861 (2)	0.0172 (11)
C11	0.5357 (3)	1.1100 (11)	0.6684 (2)	0.0182 (11)
C12	0.4950 (3)	0.9888 (12)	0.6197 (2)	0.0161 (11)
C13	0.5456 (3)	0.8001 (11)	0.5888 (2)	0.0150 (11)
S1	0.85264 (8)	0.0073 (3)	0.48739 (6)	0.0189 (3)
O1	0.8417 (2)	0.3886 (8)	0.40283 (15)	0.0173 (8)
N1	0.9806 (3)	0.3173 (10)	0.43450 (19)	0.0160 (9)
HN1	1.021 (4)	0.235 (15)	0.456 (3)	0.04 (2)*
C1	0.8953 (3)	0.2405 (12)	0.4417 (2)	0.0179 (11)
C2	0.9850 (3)	0.5192 (11)	0.3901 (2)	0.0161 (11)
C3	1.0549 (4)	0.6679 (12)	0.3661 (2)	0.0214 (12)
H3	1.115554	0.640591	0.378875	0.026*
C4	1.0309 (4)	0.8596 (12)	0.3222 (2)	0.0209 (12)
H4	1.076369	0.965301	0.304220	0.025*
C5	0.9402 (4)	0.9002 (12)	0.3038 (2)	0.0215 (12)
H5	0.926165	1.034052	0.274018	0.026*
C6	0.8718 (3)	0.7504 (12)	0.3281 (2)	0.0194 (11)
H6	0.810884	0.774932	0.315558	0.023*
C7	0.8969 (3)	0.5632 (11)	0.3715 (2)	0.0175 (11)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01571 (16)	0.01825 (18)	0.01870 (18)	0.00147 (13)	0.00332 (13)	0.00178 (14)
I2	0.02249 (18)	0.0226 (2)	0.01963 (19)	−0.00506 (14)	−0.00417 (14)	−0.00151 (15)
I3	0.01328 (16)	0.0296 (2)	0.01939 (19)	0.00433 (14)	−0.00095 (13)	0.00351 (16)
F1	0.0106 (14)	0.0263 (18)	0.0298 (18)	0.0009 (12)	−0.0040 (13)	0.0000 (15)
F2	0.0196 (15)	0.0230 (18)	0.0274 (18)	0.0043 (13)	0.0018 (13)	−0.0061 (15)
F3	0.0164 (15)	0.0279 (18)	0.0201 (16)	0.0002 (13)	−0.0031 (12)	−0.0072 (14)
C8	0.019 (3)	0.006 (2)	0.018 (3)	0.0031 (19)	−0.004 (2)	−0.002 (2)
C9	0.010 (2)	0.021 (3)	0.020 (3)	−0.001 (2)	0.001 (2)	0.007 (2)
C10	0.015 (2)	0.024 (3)	0.012 (3)	−0.003 (2)	0.000 (2)	0.001 (2)
C11	0.018 (3)	0.011 (3)	0.026 (3)	0.001 (2)	0.007 (2)	0.003 (2)
C12	0.011 (2)	0.020 (3)	0.017 (3)	−0.001 (2)	−0.001 (2)	0.002 (2)
C13	0.015 (2)	0.015 (3)	0.014 (3)	−0.0009 (19)	−0.002 (2)	0.001 (2)
S1	0.0167 (6)	0.0202 (7)	0.0200 (7)	0.0025 (5)	0.0036 (5)	0.0035 (6)
O1	0.0153 (17)	0.019 (2)	0.0177 (19)	0.0016 (14)	0.0007 (14)	0.0059 (16)

N1	0.012 (2)	0.023 (3)	0.012 (2)	0.0051 (18)	−0.0012 (17)	0.0016 (19)
C1	0.016 (2)	0.022 (3)	0.016 (3)	0.006 (2)	−0.002 (2)	−0.005 (2)
C2	0.014 (2)	0.015 (3)	0.018 (3)	0.004 (2)	−0.001 (2)	−0.004 (2)
C3	0.018 (3)	0.025 (3)	0.021 (3)	0.002 (2)	0.002 (2)	−0.001 (2)
C4	0.023 (3)	0.020 (3)	0.020 (3)	−0.002 (2)	0.011 (2)	−0.002 (2)
C5	0.037 (3)	0.017 (3)	0.011 (3)	0.004 (2)	0.003 (2)	0.002 (2)
C6	0.016 (3)	0.021 (3)	0.021 (3)	0.005 (2)	−0.002 (2)	−0.002 (2)
C7	0.018 (3)	0.014 (3)	0.020 (3)	−0.001 (2)	0.002 (2)	−0.004 (2)

Geometric parameters (Å, º)

I1—C8	2.096 (5)	O1—C7	1.387 (6)
I2—C10	2.086 (5)	N1—HN1	0.85 (7)
I3—C12	2.091 (5)	N1—C1	1.340 (7)
F1—C9	1.356 (5)	N1—C2	1.403 (7)
F2—C11	1.347 (6)	C2—C3	1.389 (8)
F3—C13	1.340 (6)	C2—C7	1.383 (7)
C8—C9	1.378 (7)	C3—H3	0.9500
C8—C13	1.392 (7)	C3—C4	1.393 (8)
C9—C10	1.378 (8)	C4—H4	0.9500
C10—C11	1.381 (7)	C4—C5	1.415 (8)
C11—C12	1.389 (7)	C5—H5	0.9500
C12—C13	1.379 (7)	C5—C6	1.377 (8)
S1—C1	1.666 (6)	C6—H6	0.9500
O1—C1	1.370 (6)	C6—C7	1.376 (8)
C9—C8—I1	122.3 (4)	O1—C1—S1	121.6 (4)
C9—C8—C13	117.1 (5)	N1—C1—S1	130.2 (4)
C13—C8—I1	120.5 (4)	N1—C1—O1	108.3 (5)
F1—C9—C8	118.4 (5)	C3—C2—N1	133.7 (5)
F1—C9—C10	118.7 (5)	C7—C2—N1	104.9 (4)
C10—C9—C8	122.9 (5)	C7—C2—C3	121.4 (5)
C9—C10—I2	122.3 (4)	C2—C3—H3	121.9
C9—C10—C11	117.7 (5)	C2—C3—C4	116.2 (5)
C11—C10—I2	120.0 (4)	C4—C3—H3	121.9
F2—C11—C10	119.0 (5)	C3—C4—H4	119.3
F2—C11—C12	118.7 (5)	C3—C4—C5	121.4 (5)
C10—C11—C12	122.4 (5)	C5—C4—H4	119.3
C11—C12—I3	122.9 (4)	C4—C5—H5	119.2
C13—C12—I3	119.8 (4)	C6—C5—C4	121.6 (5)
C13—C12—C11	117.3 (5)	C6—C5—H5	119.2
F3—C13—C8	118.6 (4)	C5—C6—H6	122.0
F3—C13—C12	118.7 (4)	C7—C6—C5	116.1 (5)
C12—C13—C8	122.7 (5)	C7—C6—H6	122.0
C1—O1—C7	107.6 (4)	C2—C7—O1	109.0 (5)
C1—N1—HN1	117 (5)	C6—C7—O1	127.6 (5)
C1—N1—C2	110.2 (4)	C6—C7—C2	123.4 (5)
C2—N1—HN1	132 (5)		

I1—C8—C9—F1	−0.7 (7)	C13—C8—C9—F1	−177.0 (5)
I1—C8—C9—C10	177.2 (4)	C13—C8—C9—C10	0.9 (8)
I1—C8—C13—F3	2.0 (7)	N1—C2—C3—C4	−178.6 (5)
I1—C8—C13—C12	−177.5 (4)	N1—C2—C7—O1	−1.3 (6)
I2—C10—C11—F2	1.5 (7)	N1—C2—C7—C6	179.5 (5)
I2—C10—C11—C12	−179.3 (4)	C1—O1—C7—C2	1.3 (6)
I3—C12—C13—F3	0.4 (7)	C1—O1—C7—C6	−179.6 (5)
I3—C12—C13—C8	179.9 (4)	C1—N1—C2—C3	179.1 (6)
F1—C9—C10—I2	−3.2 (7)	C1—N1—C2—C7	0.9 (6)
F1—C9—C10—C11	177.6 (5)	C2—N1—C1—S1	179.1 (4)
F2—C11—C12—I3	−0.1 (7)	C2—N1—C1—O1	−0.2 (6)
F2—C11—C12—C13	179.1 (5)	C2—C3—C4—C5	0.5 (8)
C8—C9—C10—I2	178.9 (4)	C3—C2—C7—O1	−179.7 (5)
C8—C9—C10—C11	−0.3 (8)	C3—C2—C7—C6	1.0 (8)
C9—C8—C13—F3	178.3 (5)	C3—C4—C5—C6	−0.6 (8)
C9—C8—C13—C12	−1.1 (8)	C4—C5—C6—C7	0.8 (8)
C9—C10—C11—F2	−179.2 (5)	C5—C6—C7—O1	179.9 (5)
C9—C10—C11—C12	−0.1 (8)	C5—C6—C7—C2	−1.1 (8)
C10—C11—C12—I3	−179.2 (4)	C7—O1—C1—S1	180.0 (4)
C10—C11—C12—C13	−0.1 (8)	C7—O1—C1—N1	−0.7 (6)
C11—C12—C13—F3	−178.7 (5)	C7—C2—C3—C4	−0.7 (8)
C11—C12—C13—C8	0.7 (8)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···S1^{i}	0.85 (7)	2.53 (7)	3.377 (4)	176 (6)
C3—H3···I1^{ii}	0.95	3.04	3.969 (5)	167
C6—H6···I2^{iii}	0.95	3.23	4.009 (5)	140

Symmetry codes: (i) −*x*+2, −*y*, −*z*+1; (ii) −*x*+2, −*y*+1, −*z*+1; (iii) *x*, −*y*+5/2, *z*−1/2.

1,3-Benzothiazole-2-thiol)–1,2,3,4-tetrafluoro-5,6-diiodobenzene (3/4) (3MBZTH_412F4DIB)

Crystal data

$4C_6F_4I_2·3C_7H_5NS_2$
M_r = 2109.16
Triclinic, $P\overline{1}$
a = 7.9410 (8) Å
b = 14.8483 (15) Å
c = 24.641 (3) Å
α = 79.264 (4)°
β = 87.104 (4)°
γ = 82.784 (4)°
V = 2830.9 (5) Å^3
Z = 2
F(000) = 1940
D_x = 2.474 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
μ = 4.69 mm^{-1}
T = 100 K
Plate, colourless
0.30 × 0.13 × 0.04 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec I*μ*S
φ and *ω* scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.570, T_{max} = 0.746
78566 measured reflections

12466 independent reflections
11325 reflections with $I > 2\sigma(I)$
$R_{int} = 0.067$
$\theta_{max} = 27.2°$, $\theta_{min} = 2.5°$
$h = -10 \rightarrow 10$
$k = -19 \rightarrow 19$
$l = -31 \rightarrow 31$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.067$
$wR(F^2) = 0.220$
$S = 1.06$
12466 reflections
704 parameters
66 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1285P)^2 + 109.2112P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 2.61$ e Å^{-3}
$\Delta\rho_{min} = -1.48$ e Å^{-3}

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. Refined as a 2-component twin.

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

	x	y	z	U_{iso}*/U_{eq}
I1	0.36226 (13)	1.16753 (7)	0.05962 (4)	0.0199 (2)
I2	−0.11193 (13)	1.17703 (7)	0.07045 (4)	0.0192 (2)
S3	0.8569 (5)	0.2851 (3)	0.27854 (18)	0.0222 (8)
S4	0.9358 (5)	0.3501 (3)	0.15807 (18)	0.0219 (8)
F1	−0.1901 (12)	0.9764 (7)	0.0748 (4)	0.023 (2)
F2	0.0046 (12)	0.8143 (6)	0.0705 (4)	0.0210 (18)
F3	0.3454 (12)	0.8083 (6)	0.0614 (4)	0.0218 (19)
F4	0.4959 (11)	0.9599 (7)	0.0585 (4)	0.023 (2)
N2	0.7575 (18)	0.4523 (10)	0.2157 (6)	0.022 (3)
HN2	0.702118	0.472763	0.243675	0.026*
C8	0.8414 (19)	0.3657 (12)	0.2214 (7)	0.022 (3)
C9	0.8613 (18)	0.4590 (11)	0.1256 (8)	0.022 (3)
C10	0.877 (2)	0.5034 (12)	0.0712 (7)	0.025 (3)
H10	0.946102	0.474610	0.045108	0.030*
C11	0.792 (3)	0.5893 (13)	0.0558 (8)	0.033 (3)
H11	0.792908	0.617175	0.017859	0.040*
C12	0.704 (2)	0.6375 (13)	0.0933 (8)	0.029 (3)
H12	0.656903	0.699744	0.081256	0.035*
C13	0.683 (2)	0.5975 (11)	0.1470 (8)	0.024 (3)
H13	0.616999	0.629053	0.172475	0.029*
C14	0.764 (2)	0.5071 (12)	0.1632 (7)	0.021 (3)
C22	0.2314 (19)	1.0522 (10)	0.0647 (6)	0.014 (3)
C23	0.0557 (18)	1.0544 (10)	0.0689 (6)	0.016 (3)
C24	−0.0213 (17)	0.9775 (10)	0.0714 (6)	0.014 (2)
C25	0.0758 (19)	0.8923 (10)	0.0684 (6)	0.015 (2)

C26	0.2483 (19)	0.8892 (10)	0.0642 (6)	0.016 (3)
C27	0.3254 (18)	0.9675 (10)	0.0619 (6)	0.015 (3)
I3	0.64678 (12)	1.13261 (7)	0.23166 (4)	0.0194 (2)
I4	0.18439 (13)	1.10869 (8)	0.23135 (5)	0.0227 (2)
F5	0.1660 (12)	0.9119 (8)	0.2046 (5)	0.028 (2)
F6	0.4004 (14)	0.7773 (7)	0.1803 (5)	0.032 (2)
F7	0.7341 (13)	0.8013 (7)	0.1742 (5)	0.028 (2)
F8	0.8342 (12)	0.9554 (7)	0.1967 (5)	0.027 (2)
C28	0.548 (2)	1.0190 (11)	0.2120 (6)	0.019 (3)
C29	0.3765 (17)	1.0068 (10)	0.2139 (6)	0.014 (3)
C30	0.3304 (19)	0.9261 (12)	0.2037 (6)	0.019 (3)
C31	0.447 (2)	0.8555 (11)	0.1910 (7)	0.020 (3)
C32	0.618 (2)	0.8672 (12)	0.1869 (7)	0.022 (3)
C33	0.6663 (18)	0.9461 (11)	0.1986 (7)	0.018 (3)
I5	0.23233 (12)	0.71859 (7)	0.32850 (4)	0.0183 (2)
I6	−0.23322 (12)	0.70593 (7)	0.32425 (4)	0.0200 (2)
F9	−0.4093 (13)	0.8951 (8)	0.3451 (4)	0.028 (2)
F10	−0.2991 (13)	1.0414 (7)	0.3748 (5)	0.028 (2)
F11	0.0385 (13)	1.0534 (7)	0.3782 (5)	0.027 (2)
F12	0.2640 (12)	0.9152 (7)	0.3547 (5)	0.026 (2)
C34	0.0485 (19)	0.8268 (10)	0.3394 (6)	0.017 (3)
C35	−0.1293 (18)	0.8223 (10)	0.3377 (6)	0.015 (2)
C36	−0.2433 (18)	0.8975 (10)	0.3469 (6)	0.016 (2)
C37	−0.1897 (18)	0.9730 (10)	0.3622 (6)	0.015 (2)
C38	−0.016 (2)	0.9776 (11)	0.3644 (7)	0.020 (3)
C39	0.097 (2)	0.9065 (10)	0.3535 (7)	0.019 (3)
I7	0.02233 (13)	0.46575 (7)	0.37019 (4)	0.0196 (2)
I8	−0.02757 (15)	0.35978 (8)	0.51719 (5)	0.0269 (3)
F13	0.1440 (16)	0.1570 (8)	0.5289 (4)	0.036 (3)
F14	0.3307 (17)	0.0627 (7)	0.4593 (5)	0.037 (3)
F15	0.3867 (14)	0.1426 (7)	0.3536 (4)	0.030 (2)
F16	0.2600 (13)	0.3180 (7)	0.3159 (4)	0.026 (2)
C40	0.1256 (19)	0.3310 (9)	0.4037 (6)	0.015 (3)
C41	0.100 (2)	0.2902 (12)	0.4582 (7)	0.020 (3)
C42	0.171 (2)	0.2029 (13)	0.4767 (7)	0.025 (3)
C43	0.263 (2)	0.1486 (12)	0.4419 (7)	0.023 (3)
C44	0.292 (2)	0.1890 (11)	0.3876 (7)	0.022 (3)
C45	0.223 (2)	0.2791 (10)	0.3680 (6)	0.017 (3)
S1	0.5243 (5)	0.5375 (3)	0.31454 (16)	0.0193 (7)
S2	0.4491 (5)	0.4693 (3)	0.43557 (17)	0.0217 (8)
N1	0.6185 (17)	0.3686 (9)	0.3737 (6)	0.020 (2)
HN1	0.671175	0.349037	0.345043	0.025*
C1	0.5386 (19)	0.4543 (10)	0.3712 (6)	0.0156 (18)
C2	0.518 (2)	0.3547 (12)	0.4654 (7)	0.022 (3)
C3	0.498 (2)	0.3107 (13)	0.5198 (6)	0.024 (3)
H3	0.442344	0.342280	0.547045	0.029*
C4	0.566 (3)	0.2171 (16)	0.5328 (9)	0.042 (5)
H4	0.548501	0.183201	0.568902	0.050*

C5	0.659 (3)	0.1730 (14)	0.4927 (8)	0.037 (5)
H5	0.705227	0.110313	0.502792	0.044*
C6	0.684 (2)	0.2196 (12)	0.4377 (8)	0.028 (4)
H6	0.746640	0.190247	0.410614	0.033*
C7	0.610 (2)	0.3135 (11)	0.4259 (8)	0.024 (3)
S5	0.5779 (5)	0.3528 (3)	0.04223 (16)	0.0185 (7)
S6	0.4242 (5)	0.3654 (3)	0.15534 (16)	0.0196 (7)
N3	0.3879 (16)	0.4977 (9)	0.0733 (5)	0.016 (2)
HN3	0.397601	0.531273	0.040138	0.019*
C15	0.4623 (19)	0.4112 (10)	0.0858 (6)	0.016 (3)
C16	0.3061 (19)	0.4678 (10)	0.1659 (6)	0.016 (3)
C17	0.216 (2)	0.4894 (11)	0.2134 (6)	0.021 (3)
H17	0.215714	0.445412	0.246790	0.025*
C18	0.128 (2)	0.5768 (12)	0.2101 (7)	0.025 (3)
H18	0.074519	0.594232	0.242502	0.030*
C19	0.116 (2)	0.6408 (11)	0.1597 (8)	0.026 (4)
H19	0.048383	0.698679	0.158241	0.032*
C20	0.2008 (19)	0.6197 (10)	0.1133 (7)	0.019 (3)
H20	0.197834	0.663313	0.079745	0.022*
C21	0.2922 (19)	0.5323 (10)	0.1166 (6)	0.015 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.0179 (5)	0.0178 (5)	0.0249 (5)	−0.0061 (4)	0.0017 (4)	−0.0046 (4)
I2	0.0168 (5)	0.0176 (4)	0.0238 (5)	0.0017 (3)	0.0003 (4)	−0.0076 (4)
S3	0.026 (2)	0.0144 (17)	0.026 (2)	0.0011 (14)	0.0023 (16)	−0.0064 (15)
S4	0.0223 (19)	0.0171 (18)	0.027 (2)	−0.0012 (14)	0.0041 (16)	−0.0092 (15)
F1	0.014 (4)	0.025 (5)	0.030 (5)	−0.001 (4)	0.001 (4)	−0.004 (4)
F2	0.021 (2)	0.022 (2)	0.022 (2)	−0.0089 (18)	−0.0027 (18)	−0.0044 (18)
F3	0.016 (4)	0.016 (4)	0.032 (5)	0.004 (3)	0.000 (4)	−0.006 (4)
F4	0.007 (4)	0.024 (5)	0.038 (6)	−0.004 (3)	0.001 (4)	−0.006 (4)
N2	0.020 (7)	0.020 (7)	0.026 (7)	0.002 (5)	0.001 (5)	−0.009 (6)
C8	0.011 (7)	0.025 (8)	0.032 (9)	−0.002 (6)	−0.011 (6)	−0.011 (7)
C9	0.004 (6)	0.021 (8)	0.043 (10)	0.000 (5)	−0.001 (6)	−0.011 (7)
C10	0.030 (7)	0.021 (7)	0.025 (7)	0.001 (6)	−0.012 (6)	−0.009 (6)
C11	0.042 (7)	0.028 (7)	0.031 (7)	0.011 (6)	−0.019 (6)	−0.013 (6)
C12	0.028 (7)	0.025 (7)	0.034 (7)	0.002 (6)	−0.010 (6)	−0.008 (6)
C13	0.012 (7)	0.019 (8)	0.041 (10)	−0.001 (6)	−0.005 (7)	−0.007 (7)
C14	0.023 (8)	0.024 (8)	0.019 (7)	−0.009 (6)	0.015 (6)	−0.010 (6)
C22	0.018 (7)	0.014 (6)	0.006 (6)	0.004 (5)	0.001 (5)	0.001 (5)
C23	0.009 (5)	0.018 (6)	0.018 (6)	0.001 (5)	0.002 (5)	−0.001 (5)
C24	0.005 (5)	0.016 (5)	0.021 (5)	0.002 (4)	0.004 (4)	−0.004 (4)
C25	0.016 (6)	0.013 (6)	0.016 (6)	0.000 (5)	0.002 (5)	−0.004 (5)
C26	0.016 (7)	0.015 (7)	0.017 (7)	0.006 (5)	−0.008 (6)	−0.008 (6)
C27	0.012 (6)	0.012 (6)	0.020 (7)	0.001 (5)	0.004 (5)	−0.005 (6)
I3	0.0164 (5)	0.0180 (5)	0.0230 (5)	−0.0020 (3)	0.0015 (4)	−0.0025 (4)
I4	0.0135 (4)	0.0257 (5)	0.0256 (5)	0.0039 (4)	0.0016 (4)	−0.0007 (4)

F5	0.010 (4)	0.041 (6)	0.036 (6)	−0.007 (4)	0.001 (4)	−0.012 (5)
F6	0.026 (5)	0.025 (5)	0.049 (7)	−0.004 (4)	−0.003 (5)	−0.013 (5)
F7	0.022 (5)	0.028 (5)	0.036 (6)	0.000 (4)	0.004 (4)	−0.015 (4)
F8	0.009 (4)	0.028 (5)	0.047 (6)	−0.003 (4)	0.001 (4)	−0.013 (5)
C28	0.019 (8)	0.017 (7)	0.016 (7)	0.001 (6)	0.008 (6)	0.001 (6)
C29	0.006 (6)	0.018 (7)	0.022 (7)	−0.003 (5)	−0.001 (5)	−0.010 (6)
C30	0.013 (7)	0.034 (9)	0.008 (6)	−0.003 (6)	−0.005 (5)	−0.001 (6)
C31	0.016 (7)	0.020 (7)	0.025 (8)	0.000 (6)	−0.005 (6)	−0.004 (6)
C32	0.020 (8)	0.027 (8)	0.021 (8)	−0.001 (6)	−0.004 (6)	−0.007 (6)
C33	0.004 (6)	0.022 (8)	0.028 (8)	−0.002 (5)	0.003 (6)	−0.007 (6)
I5	0.0127 (4)	0.0181 (4)	0.0233 (5)	0.0019 (3)	0.0022 (4)	−0.0047 (4)
I6	0.0161 (5)	0.0194 (5)	0.0249 (5)	−0.0025 (4)	−0.0033 (4)	−0.0039 (4)
F9	0.016 (5)	0.031 (5)	0.032 (5)	0.002 (4)	−0.001 (4)	0.004 (4)
F10	0.022 (5)	0.020 (5)	0.042 (6)	0.008 (4)	0.002 (4)	−0.010 (4)
F11	0.025 (5)	0.022 (5)	0.038 (6)	−0.004 (4)	−0.001 (4)	−0.013 (4)
F12	0.012 (4)	0.020 (5)	0.043 (6)	−0.002 (4)	−0.001 (4)	0.003 (4)
C34	0.014 (7)	0.008 (6)	0.023 (7)	0.003 (5)	0.003 (6)	0.007 (5)
C35	0.008 (5)	0.016 (5)	0.020 (5)	−0.001 (4)	−0.003 (4)	0.004 (4)
C36	0.006 (4)	0.017 (5)	0.020 (5)	0.001 (4)	−0.001 (4)	0.004 (4)
C37	0.006 (5)	0.017 (5)	0.021 (5)	0.001 (4)	0.001 (4)	0.001 (4)
C38	0.021 (8)	0.017 (7)	0.021 (7)	−0.001 (6)	−0.004 (6)	0.003 (6)
C39	0.027 (8)	0.010 (6)	0.019 (7)	−0.004 (6)	0.001 (6)	0.000 (5)
I7	0.0181 (5)	0.0162 (4)	0.0234 (5)	0.0003 (3)	−0.0028 (4)	−0.0016 (4)
I8	0.0288 (6)	0.0313 (6)	0.0212 (5)	−0.0007 (4)	0.0039 (4)	−0.0091 (4)
F13	0.048 (7)	0.029 (6)	0.022 (5)	−0.004 (5)	0.001 (5)	0.012 (4)
F14	0.056 (8)	0.018 (5)	0.033 (6)	0.009 (5)	−0.011 (5)	0.000 (4)
F15	0.031 (6)	0.030 (5)	0.030 (5)	0.010 (4)	0.007 (4)	−0.016 (4)
F16	0.026 (5)	0.030 (5)	0.018 (5)	0.003 (4)	0.006 (4)	0.001 (4)
C40	0.019 (7)	0.007 (6)	0.017 (7)	0.003 (5)	0.002 (5)	−0.002 (5)
C41	0.015 (6)	0.027 (7)	0.017 (6)	−0.002 (5)	−0.006 (5)	0.003 (5)
C42	0.019 (6)	0.035 (7)	0.013 (5)	0.009 (5)	0.001 (5)	0.007 (5)
C43	0.022 (6)	0.022 (7)	0.020 (6)	0.004 (6)	−0.008 (5)	0.004 (5)
C44	0.024 (8)	0.020 (8)	0.024 (8)	−0.002 (6)	0.002 (6)	−0.009 (6)
C45	0.018 (7)	0.014 (7)	0.016 (7)	0.003 (5)	0.002 (6)	0.000 (6)
S1	0.0186 (17)	0.0161 (17)	0.0224 (18)	0.0004 (14)	0.0010 (14)	−0.0038 (14)
S2	0.0197 (18)	0.0264 (19)	0.0195 (17)	0.0001 (15)	0.0006 (14)	−0.0077 (15)
N1	0.020 (5)	0.021 (5)	0.023 (5)	−0.004 (4)	−0.001 (4)	−0.007 (4)
C1	0.015 (4)	0.019 (4)	0.017 (4)	−0.006 (3)	−0.002 (3)	−0.010 (3)
C2	0.015 (7)	0.030 (9)	0.021 (8)	−0.008 (6)	0.003 (6)	−0.003 (7)
C3	0.019 (8)	0.042 (10)	0.010 (7)	−0.005 (7)	0.001 (6)	−0.001 (7)
C4	0.041 (12)	0.051 (13)	0.032 (10)	−0.030 (10)	−0.007 (9)	0.011 (9)
C5	0.058 (13)	0.026 (9)	0.022 (9)	−0.008 (9)	−0.008 (8)	0.010 (7)
C6	0.031 (9)	0.018 (8)	0.033 (9)	−0.004 (7)	−0.012 (7)	0.001 (7)
C7	0.026 (8)	0.014 (7)	0.031 (9)	−0.002 (6)	−0.009 (7)	0.002 (6)
S5	0.0195 (18)	0.0119 (16)	0.0226 (18)	0.0032 (13)	0.0020 (14)	−0.0028 (14)
S6	0.0213 (18)	0.0154 (17)	0.0201 (18)	0.0013 (14)	−0.0005 (14)	−0.0005 (14)
N3	0.016 (6)	0.014 (6)	0.017 (6)	0.004 (5)	0.000 (5)	−0.003 (5)
C15	0.018 (7)	0.011 (6)	0.020 (7)	−0.002 (5)	−0.007 (6)	−0.001 (5)

C16	0.013 (7)	0.015 (7)	0.019 (7)	−0.001 (5)	0.002 (5)	−0.002 (6)
C17	0.031 (9)	0.021 (8)	0.009 (6)	0.001 (7)	−0.003 (6)	0.002 (6)
C18	0.016 (7)	0.030 (9)	0.028 (8)	0.004 (6)	0.001 (6)	−0.009 (7)
C19	0.033 (9)	0.012 (7)	0.033 (9)	0.007 (6)	−0.006 (7)	−0.008 (7)
C20	0.016 (7)	0.014 (7)	0.024 (8)	−0.005 (6)	0.013 (6)	0.000 (6)
C21	0.018 (7)	0.012 (6)	0.016 (7)	−0.005 (5)	0.004 (5)	−0.004 (5)

Geometric parameters (Å, º)

I1—C22	2.094 (15)	C35—C36	1.39 (2)
I2—C23	2.121 (15)	C36—C37	1.37 (2)
S3—C8	1.669 (18)	C37—C38	1.40 (2)
S4—C8	1.738 (18)	C38—C39	1.35 (2)
S4—C9	1.711 (17)	I7—C40	2.097 (14)
F1—C24	1.341 (16)	I8—C41	2.086 (17)
F2—C25	1.344 (17)	F13—C42	1.358 (19)
F3—C26	1.355 (16)	F14—C43	1.320 (19)
F4—C27	1.344 (17)	F15—C44	1.328 (18)
N2—HN2	0.8800	F16—C45	1.341 (18)
N2—C8	1.36 (2)	C40—C41	1.38 (2)
N2—C14	1.40 (2)	C40—C45	1.41 (2)
C9—C10	1.39 (3)	C41—C42	1.35 (2)
C9—C14	1.42 (2)	C42—C43	1.40 (2)
C10—H10	0.9500	C43—C44	1.38 (2)
C10—C11	1.36 (2)	C44—C45	1.39 (2)
C11—H11	0.9500	S1—C1	1.680 (16)
C11—C12	1.38 (3)	S2—C1	1.747 (15)
C12—H12	0.9500	S2—C2	1.755 (19)
C12—C13	1.36 (3)	N1—HN1	0.8800
C13—H13	0.9500	N1—C1	1.34 (2)
C13—C14	1.41 (2)	N1—C7	1.39 (2)
C22—C23	1.39 (2)	C2—C3	1.39 (2)
C22—C27	1.391 (19)	C2—C7	1.38 (2)
C23—C24	1.35 (2)	C3—H3	0.9500
C24—C25	1.408 (19)	C3—C4	1.41 (3)
C25—C26	1.36 (2)	C4—H4	0.9500
C26—C27	1.37 (2)	C4—C5	1.41 (3)
I3—C28	2.089 (16)	C5—H5	0.9500
I4—C29	2.097 (14)	C5—C6	1.42 (3)
F5—C30	1.347 (18)	C6—H6	0.9500
F6—C31	1.336 (19)	C6—C7	1.43 (2)
F7—C32	1.330 (19)	S5—C15	1.671 (16)
F8—C33	1.355 (17)	S6—C15	1.749 (16)
C28—C29	1.40 (2)	S6—C16	1.740 (15)
C28—C33	1.42 (2)	N3—HN3	0.8800
C29—C30	1.37 (2)	N3—C15	1.331 (19)
C30—C31	1.38 (2)	N3—C21	1.416 (19)
C31—C32	1.38 (2)	C16—C17	1.41 (2)

C32—C33	1.36 (2)	C16—C21	1.40 (2)
I5—C34	2.077 (14)	C17—H17	0.9500
I6—C35	2.092 (15)	C17—C18	1.38 (2)
F9—C36	1.326 (17)	C18—H18	0.9500
F10—C37	1.323 (17)	C18—C19	1.41 (3)
F11—C38	1.359 (19)	C19—H19	0.9500
F12—C39	1.348 (19)	C19—C20	1.36 (2)
C34—C35	1.43 (2)	C20—H20	0.9500
C34—C39	1.40 (2)	C20—C21	1.40 (2)

C9—S4—C8	93.5 (8)	C39—C38—F11	120.7 (15)
C8—N2—HN2	121.8	C39—C38—C37	120.0 (15)
C8—N2—C14	116.5 (14)	F12—C39—C34	119.1 (14)
C14—N2—HN2	121.8	F12—C39—C38	117.8 (14)
S3—C8—S4	123.8 (10)	C38—C39—C34	123.1 (16)
N2—C8—S3	127.4 (14)	C41—C40—I7	123.4 (11)
N2—C8—S4	108.8 (13)	C41—C40—C45	118.8 (14)
C10—C9—S4	131.6 (13)	C45—C40—I7	117.7 (11)
C10—C9—C14	118.2 (15)	C40—C41—I8	123.5 (12)
C14—C9—S4	110.2 (14)	C42—C41—I8	116.4 (12)
C9—C10—H10	120.7	C42—C41—C40	119.9 (15)
C11—C10—C9	118.6 (17)	F13—C42—C43	114.0 (15)
C11—C10—H10	120.7	C41—C42—F13	123.0 (15)
C10—C11—H11	118.7	C41—C42—C43	122.7 (15)
C10—C11—C12	122.6 (19)	F14—C43—C42	123.2 (15)
C12—C11—H11	118.7	F14—C43—C44	118.8 (16)
C11—C12—H12	119.4	C44—C43—C42	117.9 (15)
C13—C12—C11	121.1 (18)	F15—C44—C43	120.7 (15)
C13—C12—H12	119.4	F15—C44—C45	119.1 (15)
C12—C13—H13	121.5	C43—C44—C45	120.3 (15)
C12—C13—C14	116.9 (16)	F16—C45—C40	120.7 (13)
C14—C13—H13	121.5	F16—C45—C44	118.9 (14)
N2—C14—C9	111.1 (15)	C44—C45—C40	120.3 (14)
N2—C14—C13	126.8 (15)	C1—S2—C2	92.1 (8)
C13—C14—C9	122.1 (16)	C1—N1—HN1	123.1
C23—C22—I1	124.6 (10)	C1—N1—C7	113.8 (14)
C23—C22—C27	117.2 (14)	C7—N1—HN1	123.1
C27—C22—I1	118.1 (11)	S1—C1—S2	123.6 (9)
C22—C23—I2	123.4 (11)	N1—C1—S1	125.7 (12)
C24—C23—I2	114.8 (10)	N1—C1—S2	110.7 (12)
C24—C23—C22	121.8 (14)	C3—C2—S2	128.6 (14)
F1—C24—C23	123.9 (13)	C7—C2—S2	108.1 (12)
F1—C24—C25	115.8 (13)	C7—C2—C3	123.1 (17)
C23—C24—C25	120.3 (13)	C2—C3—H3	121.6
F2—C25—C24	122.3 (13)	C2—C3—C4	116.9 (17)
F2—C25—C26	119.2 (13)	C4—C3—H3	121.6
C26—C25—C24	118.5 (13)	C3—C4—H4	119.6
F3—C26—C25	120.0 (13)	C3—C4—C5	120.8 (17)

F3—C26—C27	119.2 (13)	C5—C4—H4	119.6
C25—C26—C27	120.8 (13)	C4—C5—H5	119.0
F4—C27—C22	120.4 (13)	C4—C5—C6	122.0 (19)
F4—C27—C26	118.2 (13)	C6—C5—H5	119.0
C26—C27—C22	121.4 (14)	C5—C6—H6	122.2
C29—C28—I3	125.4 (11)	C5—C6—C7	115.5 (18)
C29—C28—C33	117.2 (14)	C7—C6—H6	122.2
C33—C28—I3	117.3 (11)	N1—C7—C6	123.2 (17)
C28—C29—I4	122.4 (11)	C2—C7—N1	115.2 (15)
C30—C29—I4	118.3 (10)	C2—C7—C6	121.5 (17)
C30—C29—C28	119.3 (14)	C16—S6—C15	91.6 (7)
F5—C30—C29	121.1 (14)	C15—N3—HN3	122.0
F5—C30—C31	116.1 (15)	C15—N3—C21	116.0 (13)
C29—C30—C31	122.7 (14)	C21—N3—HN3	122.0
F6—C31—C30	122.3 (14)	S5—C15—S6	123.6 (9)
F6—C31—C32	118.6 (15)	N3—C15—S5	125.8 (12)
C30—C31—C32	119.1 (15)	N3—C15—S6	110.6 (12)
F7—C32—C31	121.1 (15)	C17—C16—S6	129.9 (12)
F7—C32—C33	119.9 (14)	C21—C16—S6	110.9 (11)
C33—C32—C31	119.0 (15)	C21—C16—C17	118.9 (14)
F8—C33—C28	118.8 (14)	C16—C17—H17	121.0
F8—C33—C32	118.6 (14)	C18—C17—C16	117.9 (15)
C32—C33—C28	122.6 (14)	C18—C17—H17	121.0
C35—C34—I5	123.6 (11)	C17—C18—H18	119.0
C39—C34—I5	119.6 (11)	C17—C18—C19	121.9 (15)
C39—C34—C35	116.6 (14)	C19—C18—H18	119.0
C34—C35—I6	123.6 (11)	C18—C19—H19	119.9
C36—C35—I6	116.8 (10)	C20—C19—C18	120.3 (15)
C36—C35—C34	119.6 (14)	C20—C19—H19	119.9
F9—C36—C35	120.7 (14)	C19—C20—H20	121.0
F9—C36—C37	117.6 (13)	C19—C20—C21	118.0 (15)
C37—C36—C35	121.5 (13)	C21—C20—H20	121.0
F10—C37—C36	121.4 (13)	C16—C21—N3	110.8 (13)
F10—C37—C38	119.6 (14)	C20—C21—N3	126.5 (14)
C36—C37—C38	119.0 (14)	C20—C21—C16	122.6 (14)
F11—C38—C37	119.3 (14)		

I1—C22—C23—I2	0.4 (18)	F11—C38—C39—F12	−3 (2)
I1—C22—C23—C24	179.1 (11)	F11—C38—C39—C34	179.7 (14)
I1—C22—C27—F4	2.9 (19)	C34—C35—C36—F9	179.6 (14)
I1—C22—C27—C26	−179.1 (11)	C34—C35—C36—C37	−6 (2)
I2—C23—C24—F1	0 (2)	C35—C34—C39—F12	−178.7 (13)
I2—C23—C24—C25	177.4 (11)	C35—C34—C39—C38	−1 (2)
S4—C9—C10—C11	174.9 (14)	C35—C36—C37—F10	−175.0 (14)
S4—C9—C14—N2	0.4 (17)	C35—C36—C37—C38	5 (2)
S4—C9—C14—C13	−178.2 (13)	C36—C37—C38—F11	178.3 (14)
F1—C24—C25—F2	−2 (2)	C36—C37—C38—C39	−3 (2)
F1—C24—C25—C26	179.3 (13)	C37—C38—C39—F12	178.2 (14)

F2—C25—C26—F3	1 (2)	C37—C38—C39—C34	1 (2)
F2—C25—C26—C27	179.9 (13)	C39—C34—C35—I6	−174.6 (11)
F3—C26—C27—F4	−2 (2)	C39—C34—C35—C36	3 (2)
F3—C26—C27—C22	−179.9 (13)	I7—C40—C41—I8	−5.3 (19)
C8—S4—C9—C10	−178.3 (16)	I7—C40—C41—C42	179.9 (13)
C8—S4—C9—C14	−0.2 (12)	I7—C40—C45—F16	6 (2)
C8—N2—C14—C9	−1 (2)	I7—C40—C45—C44	−178.8 (12)
C8—N2—C14—C13	178.0 (16)	I8—C41—C42—F13	8 (2)
C9—S4—C8—S3	−179.6 (10)	I8—C41—C42—C43	−178.7 (14)
C9—S4—C8—N2	−0.1 (12)	F13—C42—C43—F14	−5 (3)
C9—C10—C11—C12	6 (3)	F13—C42—C43—C44	178.0 (15)
C10—C9—C14—N2	178.8 (14)	F14—C43—C44—F15	−1 (3)
C10—C9—C14—C13	0 (2)	F14—C43—C44—C45	−179.9 (15)
C10—C11—C12—C13	−7 (3)	F15—C44—C45—F16	−3 (2)
C11—C12—C13—C14	4 (3)	F15—C44—C45—C40	−178.3 (15)
C12—C13—C14—N2	−178.8 (16)	C40—C41—C42—F13	−176.5 (16)
C12—C13—C14—C9	0 (2)	C40—C41—C42—C43	−4 (3)
C14—N2—C8—S3	179.9 (12)	C41—C40—C45—F16	−175.7 (14)
C14—N2—C8—S4	0.4 (17)	C41—C40—C45—C44	0 (2)
C14—C9—C10—C11	−3 (2)	C41—C42—C43—F14	−178.9 (17)
C22—C23—C24—F1	−179.2 (14)	C41—C42—C43—C44	4 (3)
C22—C23—C24—C25	−1 (2)	C42—C43—C44—F15	176.2 (16)
C23—C22—C27—F4	−179.1 (13)	C42—C43—C44—C45	−3 (3)
C23—C22—C27—C26	−1 (2)	C43—C44—C45—F16	176.8 (15)
C23—C24—C25—F2	−179.8 (14)	C43—C44—C45—C40	1 (2)
C23—C24—C25—C26	1 (2)	C45—C40—C41—I8	176.1 (11)
C24—C25—C26—F3	179.9 (13)	C45—C40—C41—C42	1 (2)
C24—C25—C26—C27	−1 (2)	S2—C2—C3—C4	179.7 (14)
C25—C26—C27—F4	179.1 (14)	S2—C2—C7—N1	−3.3 (18)
C25—C26—C27—C22	1 (2)	S2—C2—C7—C6	179.8 (14)
C27—C22—C23—I2	−177.4 (11)	C1—S2—C2—C3	178.1 (16)
C27—C22—C23—C24	1 (2)	C1—S2—C2—C7	2.8 (13)
I3—C28—C29—I4	5.1 (19)	C1—N1—C7—C2	2 (2)
I3—C28—C29—C30	−175.4 (11)	C1—N1—C7—C6	179.0 (15)
I3—C28—C33—F8	−3 (2)	C2—S2—C1—S1	178.3 (10)
I3—C28—C33—C32	177.7 (13)	C2—S2—C1—N1	−1.8 (12)
I4—C29—C30—F5	0 (2)	C2—C3—C4—C5	4 (3)
I4—C29—C30—C31	179.0 (12)	C3—C2—C7—N1	−178.9 (15)
F5—C30—C31—F6	0 (2)	C3—C2—C7—C6	4 (3)
F5—C30—C31—C32	177.2 (14)	C3—C4—C5—C6	−2 (3)
F6—C31—C32—F7	−2 (2)	C4—C5—C6—C7	0 (3)
F6—C31—C32—C33	−179.0 (15)	C5—C6—C7—N1	−177.9 (17)
F7—C32—C33—F8	0 (2)	C5—C6—C7—C2	−1 (3)
F7—C32—C33—C28	179.6 (15)	C7—N1—C1—S1	−179.9 (12)
C28—C29—C30—F5	−179.4 (14)	C7—N1—C1—S2	0.2 (16)
C28—C29—C30—C31	0 (2)	C7—C2—C3—C4	−6 (3)
C29—C28—C33—F8	−179.5 (14)	S6—C16—C17—C18	−178.4 (13)
C29—C28—C33—C32	1 (2)	S6—C16—C21—N3	−4.0 (16)

C29—C30—C31—F6	−179.1 (15)	S6—C16—C21—C20	178.7 (12)
C29—C30—C31—C32	−2 (2)	C15—S6—C16—C17	176.4 (16)
C30—C31—C32—F7	−179.3 (15)	C15—S6—C16—C21	2.5 (12)
C30—C31—C32—C33	4 (2)	C15—N3—C21—C16	4.0 (19)
C31—C32—C33—F8	177.3 (15)	C15—N3—C21—C20	−178.8 (15)
C31—C32—C33—C28	−3 (3)	C16—S6—C15—S5	179.3 (10)
C33—C28—C29—I4	−178.6 (11)	C16—S6—C15—N3	−0.3 (12)
C33—C28—C29—C30	1 (2)	C16—C17—C18—C19	5 (3)
I5—C34—C35—I6	0.3 (19)	C17—C16—C21—N3	−178.6 (14)
I5—C34—C35—C36	178.4 (11)	C17—C16—C21—C20	4 (2)
I5—C34—C39—F12	6 (2)	C17—C18—C19—C20	−4 (3)
I5—C34—C39—C38	−176.1 (12)	C18—C19—C20—C21	3 (3)
I6—C35—C36—F9	−2.2 (19)	C19—C20—C21—N3	−180.0 (15)
I6—C35—C36—C37	172.5 (12)	C19—C20—C21—C16	−3 (2)
F9—C36—C37—F10	0 (2)	C21—N3—C15—S5	178.4 (11)
F9—C36—C37—C38	−179.9 (14)	C21—N3—C15—S6	−2.0 (17)
F10—C37—C38—F11	−1 (2)	C21—C16—C17—C18	−5 (2)
F10—C37—C38—C39	177.6 (15)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H*N*2···S1	0.88	2.45	3.326 (14)	174
N1—H*N*1···S3	0.88	2.40	3.266 (14)	169
C6—H6···F10^{i}	0.95	2.60	3.29 (2)	130
N3—H*N*3···S5^{ii}	0.88	2.42	3.290 (14)	170
C17—H17···F16	0.95	2.30	3.232 (18)	166
C20—H20···F2	0.95	2.53	3.128 (18)	121
C20—H20···F3	0.95	2.54	3.181 (17)	125

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

1,3-Benzothiazole-2-thiol–1,2,3,5-tetrafluoro-4,6-diiodobenzene (1/1) (MBZTH_13F4DIB)

Crystal data

$C_6F_4I_2·C_7H_5NS_2$
M_r = 569.10
Triclinic, $P\overline{1}$
a = 7.2175 (4) Å
b = 8.2675 (5) Å
c = 14.4498 (9) Å
α = 97.936 (2)°
β = 91.297 (2)°
γ = 109.178 (2)°
V = 804.44 (8) Å^3
Z = 2
$F(000)$ = 528
D_x = 2.349 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9969 reflections
θ = 2.6–30.1°
μ = 4.20 mm^{-1}
T = 100 K
Plate, colourless
0.33 × 0.27 × 0.06 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec IμS
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.496, T_{max} = 0.746
27899 measured reflections

4701 independent reflections
4391 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 30.1°$, $\theta_{min} = 2.6°$
$h = -10 \rightarrow 10$
$k = -11 \rightarrow 11$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.018$
$wR(F^2) = 0.044$
$S = 1.09$
4701 reflections
203 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0115P)^2 + 0.801P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 1.08$ e Å^{-3}
$\Delta\rho_{min} = -1.11$ e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.21928 (2)	0.04578 (2)	0.73577 (2)	0.02046 (4)
I2	0.40359 (2)	0.24728 (2)	0.35536 (2)	0.02203 (4)
F1	0.17793 (18)	0.11993 (18)	0.52937 (9)	0.0275 (3)
F2	0.83758 (19)	0.35764 (19)	0.45929 (9)	0.0317 (3)
F3	0.95882 (18)	0.33437 (18)	0.63449 (9)	0.0304 (3)
F4	0.69486 (18)	0.19590 (15)	0.75449 (8)	0.0219 (2)
C8	0.4287 (3)	0.1563 (2)	0.64457 (13)	0.0174 (3)
C9	0.3711 (3)	0.1745 (3)	0.55526 (13)	0.0192 (4)
C10	0.5038 (3)	0.2421 (2)	0.49121 (13)	0.0184 (3)
C11	0.7028 (3)	0.2946 (3)	0.51885 (14)	0.0207 (4)
C12	0.7664 (3)	0.2813 (3)	0.60795 (14)	0.0209 (4)
C13	0.6289 (3)	0.2109 (2)	0.66928 (12)	0.0180 (3)
S1	0.82694 (7)	0.91230 (6)	0.86324 (3)	0.01549 (8)
S2	0.65916 (6)	0.53019 (5)	0.86630 (3)	0.01339 (8)
N1	0.8612 (2)	0.74012 (19)	1.00562 (10)	0.0127 (3)
HN1	0.938 (4)	0.835 (4)	1.0386 (19)	0.027 (7)*
C1	0.7938 (2)	0.7398 (2)	0.91829 (12)	0.0126 (3)
C2	0.7006 (2)	0.4453 (2)	0.96579 (12)	0.0127 (3)
C3	0.6389 (3)	0.2736 (2)	0.98130 (13)	0.0165 (3)
H3	0.563536	0.182216	0.934125	0.020*
C4	0.6913 (3)	0.2405 (2)	1.06823 (14)	0.0185 (3)
H4	0.650289	0.124547	1.080638	0.022*
C5	0.8032 (3)	0.3749 (2)	1.13778 (13)	0.0172 (3)
H5	0.836221	0.348582	1.196613	0.021*
C6	0.8667 (3)	0.5457 (2)	1.12210 (13)	0.0150 (3)
H6	0.943886	0.636838	1.168951	0.018*

C7	0.8134 (2)	0.5792 (2)	1.03532 (12)	0.0128 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.02600 (7)	0.02230 (6)	0.01536 (6)	0.00997 (5)	0.00446 (4)	0.00537 (4)
I2	0.03060 (7)	0.02527 (7)	0.01257 (6)	0.01186 (5)	−0.00081 (5)	0.00492 (4)
F1	0.0198 (6)	0.0426 (7)	0.0197 (6)	0.0086 (5)	−0.0015 (4)	0.0078 (5)
F2	0.0252 (6)	0.0391 (7)	0.0221 (6)	−0.0032 (5)	0.0029 (5)	0.0105 (5)
F3	0.0199 (6)	0.0372 (7)	0.0270 (7)	0.0003 (5)	−0.0064 (5)	0.0059 (5)
F4	0.0294 (6)	0.0222 (6)	0.0134 (5)	0.0085 (5)	−0.0059 (4)	0.0017 (4)
C8	0.0223 (9)	0.0171 (8)	0.0132 (8)	0.0072 (7)	0.0010 (6)	0.0024 (6)
C9	0.0202 (9)	0.0214 (9)	0.0149 (8)	0.0064 (7)	−0.0019 (6)	0.0009 (7)
C10	0.0242 (9)	0.0171 (8)	0.0126 (8)	0.0055 (7)	−0.0027 (7)	0.0023 (6)
C11	0.0232 (9)	0.0190 (9)	0.0163 (9)	0.0019 (7)	0.0018 (7)	0.0037 (7)
C12	0.0196 (9)	0.0196 (9)	0.0194 (9)	0.0020 (7)	−0.0037 (7)	0.0020 (7)
C13	0.0275 (9)	0.0147 (8)	0.0107 (8)	0.0066 (7)	−0.0029 (7)	−0.0005 (6)
S1	0.0184 (2)	0.01360 (18)	0.01265 (19)	0.00228 (15)	−0.00070 (15)	0.00408 (15)
S2	0.01404 (19)	0.01277 (18)	0.01164 (18)	0.00286 (14)	−0.00167 (14)	0.00058 (14)
N1	0.0128 (7)	0.0128 (6)	0.0110 (6)	0.0022 (5)	−0.0004 (5)	0.0018 (5)
C1	0.0124 (7)	0.0134 (7)	0.0117 (7)	0.0041 (6)	0.0017 (6)	0.0017 (6)
C2	0.0105 (7)	0.0143 (7)	0.0137 (7)	0.0044 (6)	0.0014 (6)	0.0029 (6)
C3	0.0145 (8)	0.0126 (7)	0.0209 (9)	0.0030 (6)	0.0001 (6)	0.0021 (6)
C4	0.0183 (8)	0.0150 (8)	0.0232 (9)	0.0052 (7)	0.0026 (7)	0.0073 (7)
C5	0.0158 (8)	0.0205 (8)	0.0184 (8)	0.0078 (7)	0.0020 (6)	0.0082 (7)
C6	0.0116 (7)	0.0184 (8)	0.0158 (8)	0.0055 (6)	0.0003 (6)	0.0039 (6)
C7	0.0115 (7)	0.0128 (7)	0.0142 (8)	0.0038 (6)	0.0018 (6)	0.0026 (6)

Geometric parameters (Å, º)

I1—C8	2.0910 (19)	S2—C2	1.7452 (18)
I2—C10	2.0875 (18)	N1—HN1	0.87 (3)
F1—C9	1.343 (2)	N1—C1	1.342 (2)
F2—C11	1.337 (2)	N1—C7	1.391 (2)
F3—C12	1.341 (2)	C2—C3	1.393 (2)
F4—C13	1.346 (2)	C2—C7	1.401 (2)
C8—C9	1.390 (3)	C3—H3	0.9500
C8—C13	1.387 (3)	C3—C4	1.392 (3)
C9—C10	1.385 (3)	C4—H4	0.9500
C10—C11	1.388 (3)	C4—C5	1.401 (3)
C11—C12	1.388 (3)	C5—H5	0.9500
C12—C13	1.383 (3)	C5—C6	1.387 (3)
S1—C1	1.6799 (18)	C6—H6	0.9500
S2—C1	1.7355 (18)	C6—C7	1.393 (2)
C9—C8—I1	120.65 (14)	S1—C1—S2	122.60 (10)
C13—C8—I1	122.00 (14)	N1—C1—S1	127.05 (13)
C13—C8—C9	117.34 (18)	N1—C1—S2	110.35 (13)

F1—C9—C8	118.30 (18)	C3—C2—S2	129.26 (14)
F1—C9—C10	118.70 (17)	C3—C2—C7	120.78 (16)
C10—C9—C8	122.97 (18)	C7—C2—S2	109.95 (13)
C9—C10—I2	120.15 (14)	C2—C3—H3	121.1
C9—C10—C11	117.73 (17)	C4—C3—C2	117.77 (17)
C11—C10—I2	121.99 (14)	C4—C3—H3	121.1
F2—C11—C10	120.33 (17)	C3—C4—H4	119.4
F2—C11—C12	118.58 (18)	C3—C4—C5	121.28 (17)
C12—C11—C10	121.09 (18)	C5—C4—H4	119.4
F3—C12—C11	120.72 (18)	C4—C5—H5	119.5
F3—C12—C13	120.01 (17)	C6—C5—C4	121.03 (17)
C13—C12—C11	119.27 (18)	C6—C5—H5	119.5
F4—C13—C8	120.41 (17)	C5—C6—H6	121.1
F4—C13—C12	118.00 (17)	C5—C6—C7	117.75 (16)
C12—C13—C8	121.59 (17)	C7—C6—H6	121.1
C1—S2—C2	91.89 (8)	N1—C7—C2	111.76 (15)
C1—N1—HN1	120.5 (18)	N1—C7—C6	126.87 (16)
C1—N1—C7	116.05 (15)	C6—C7—C2	121.37 (16)
C7—N1—HN1	123.3 (18)		

I1—C8—C9—F1	0.2 (2)	C13—C8—C9—F1	178.96 (17)
I1—C8—C9—C10	−178.06 (15)	C13—C8—C9—C10	0.7 (3)
I1—C8—C13—F4	−0.8 (2)	S2—C2—C3—C4	−179.54 (14)
I1—C8—C13—C12	178.95 (15)	S2—C2—C7—N1	−0.38 (18)
I2—C10—C11—F2	2.8 (3)	S2—C2—C7—C6	179.86 (13)
I2—C10—C11—C12	−176.43 (15)	C1—S2—C2—C3	−179.18 (17)
F1—C9—C10—I2	−2.9 (3)	C1—S2—C2—C7	0.60 (13)
F1—C9—C10—C11	−178.78 (18)	C1—N1—C7—C2	−0.2 (2)
F2—C11—C12—F3	1.6 (3)	C1—N1—C7—C6	179.60 (17)
F2—C11—C12—C13	−177.81 (18)	C2—S2—C1—S1	179.93 (12)
F3—C12—C13—F4	−0.9 (3)	C2—S2—C1—N1	−0.69 (13)
F3—C12—C13—C8	179.31 (17)	C2—C3—C4—C5	−0.4 (3)
C8—C9—C10—I2	175.43 (15)	C3—C2—C7—N1	179.42 (15)
C8—C9—C10—C11	−0.5 (3)	C3—C2—C7—C6	−0.3 (3)
C9—C8—C13—F4	−179.55 (16)	C3—C4—C5—C6	−0.4 (3)
C9—C8—C13—C12	0.2 (3)	C4—C5—C6—C7	0.7 (3)
C9—C10—C11—F2	178.66 (18)	C5—C6—C7—N1	179.90 (17)
C9—C10—C11—C12	−0.6 (3)	C5—C6—C7—C2	−0.4 (3)
C10—C11—C12—F3	−179.14 (18)	C7—N1—C1—S1	179.95 (13)
C10—C11—C12—C13	1.5 (3)	C7—N1—C1—S2	0.61 (19)
C11—C12—C13—F4	178.52 (17)	C7—C2—C3—C4	0.7 (3)
C11—C12—C13—C8	−1.3 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···S1^{i}	0.87 (3)	2.45 (3)	3.3120 (15)	175 (2)

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

1,3-Benzothiazole-2-thiol–1,2,3,5-tetrafluoro-4,6-diiodobenzene (1/2) (MBZTH_213F4DIB)

Crystal data

$4C_6F_4I_2{\cdot}2C_7H_5NS_2$
M_r = 1941.92
Monoclinic, $P2_1$
a = 4.5581 (3) Å
b = 34.358 (2) Å
c = 15.6075 (10) Å
β = 94.707 (2)°
V = 2436.0 (3) Å^3
Z = 2
$F(000)$ = 1768
D_x = 2.647 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9841 reflections
θ = 2.4–28.8°
μ = 5.36 mm^{-1}
T = 100 K
Prism, colourless
0.18 × 0.12 × 0.04 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec IμS
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.568, T_{max} = 0.746
56285 measured reflections
12660 independent reflections
11766 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 28.8°, θ_{min} = 2.2°
h = −6→6
k = −46→46
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.046
S = 1.09
12660 reflections
622 parameters
2 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0071P)^2 + 0.5877P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 1.01 e Å^{-3}
$\Delta\rho_{min}$ = −0.71 e Å^{-3}
Absolute structure: Refined as an inversion twin
Absolute structure parameter: 0.454 (15)

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. Refined as a 2-component inversion twin.

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

	x	y	z	U_{iso}*/U_{eq}
I1	1.31057 (9)	0.37856 (2)	0.44709 (3)	0.01694 (9)
I2	0.58291 (10)	0.34353 (2)	0.11336 (3)	0.02224 (10)
I3	0.13207 (9)	0.44552 (2)	0.04395 (3)	0.01659 (9)
I4	0.84342 (11)	0.47934 (2)	0.38106 (3)	0.02660 (11)
F1	1.0269 (9)	0.38363 (11)	0.2525 (2)	0.0233 (9)
F2	0.4263 (9)	0.27169 (12)	0.2331 (3)	0.0284 (10)

F3	0.6051 (10)	0.25383 (12)	0.3971 (3)	0.0324 (10)
F4	0.9918 (10)	0.29933 (12)	0.4890 (2)	0.0276 (10)
F5	0.3945 (8)	0.44111 (11)	0.2407 (2)	0.0205 (8)
F6	1.0552 (9)	0.54664 (12)	0.2573 (3)	0.0301 (10)
F7	0.9034 (9)	0.56331 (12)	0.0915 (3)	0.0331 (10)
F8	0.4927 (9)	0.52114 (12)	0.0003 (2)	0.0247 (9)
C15	1.0262 (13)	0.34210 (19)	0.3717 (4)	0.0147 (13)
C16	0.9275 (14)	0.35093 (18)	0.2876 (4)	0.0163 (13)
C17	0.7260 (13)	0.32806 (19)	0.2383 (4)	0.0150 (13)
C18	0.6246 (14)	0.2950 (2)	0.2766 (4)	0.0181 (14)
C19	0.7144 (15)	0.2853 (2)	0.3607 (4)	0.0197 (14)
C20	0.9139 (15)	0.3087 (2)	0.4070 (4)	0.0187 (14)
C21	0.4273 (13)	0.48043 (17)	0.1192 (4)	0.0118 (12)
C22	0.5141 (14)	0.47193 (19)	0.2048 (4)	0.0160 (13)
C23	0.7212 (14)	0.49397 (19)	0.2538 (4)	0.0170 (13)
C24	0.8475 (14)	0.5248 (2)	0.2137 (5)	0.0204 (15)
C25	0.7690 (15)	0.53442 (19)	0.1293 (5)	0.0207 (15)
C26	0.5582 (14)	0.51219 (19)	0.0829 (4)	0.0164 (13)
I5	0.60231 (10)	0.58298 (2)	0.42231 (3)	0.02666 (11)
I6	−0.04120 (12)	0.67426 (2)	0.67979 (3)	0.03213 (12)
F13	0.3626 (9)	0.61104 (13)	0.5966 (2)	0.0298 (9)
F14	−0.1966 (10)	0.72120 (12)	0.5061 (3)	0.0340 (11)
F15	−0.0233 (11)	0.71370 (13)	0.3475 (3)	0.0379 (11)
F16	0.3387 (10)	0.65460 (13)	0.3104 (3)	0.0340 (10)
C33	0.3592 (15)	0.63148 (19)	0.4533 (4)	0.0215 (14)
C34	0.2700 (15)	0.63678 (19)	0.5348 (4)	0.0212 (14)
C35	0.0859 (15)	0.6674 (2)	0.5562 (4)	0.0215 (15)
C36	−0.0098 (16)	0.6922 (2)	0.4907 (5)	0.0241 (15)
C37	0.0756 (16)	0.6885 (2)	0.4086 (5)	0.0267 (16)
C38	0.2587 (16)	0.6584 (2)	0.3901 (4)	0.0241 (15)
I7	0.27675 (10)	0.60812 (2)	−0.10563 (3)	0.02281 (10)
I8	1.08854 (10)	0.74677 (2)	−0.05335 (3)	0.02152 (10)
F9	0.6582 (9)	0.68287 (11)	−0.1413 (2)	0.0239 (9)
F10	1.0852 (9)	0.71219 (12)	0.1364 (2)	0.0286 (10)
F11	0.7847 (10)	0.65341 (14)	0.2015 (2)	0.0365 (11)
F12	0.4105 (9)	0.61029 (12)	0.0985 (3)	0.0293 (9)
C27	0.5318 (14)	0.64475 (18)	−0.0249 (4)	0.0164 (13)
C28	0.6884 (14)	0.67579 (19)	−0.0565 (4)	0.0166 (13)
C29	0.8730 (13)	0.69920 (18)	−0.0044 (4)	0.0165 (13)
C30	0.9054 (15)	0.6911 (2)	0.0830 (4)	0.0219 (15)
C31	0.7507 (16)	0.6609 (2)	0.1168 (4)	0.0233 (15)
C32	0.5630 (14)	0.63862 (19)	0.0628 (4)	0.0202 (14)
S1	0.6754 (4)	0.40568 (5)	0.88863 (11)	0.0189 (3)
S2	1.0703 (4)	0.33606 (5)	0.91405 (10)	0.0186 (3)
N1	0.9694 (12)	0.36855 (16)	0.7688 (3)	0.0152 (11)
HN1	0.905 (14)	0.3871 (19)	0.732 (4)	0.007 (16)*
C1	0.8985 (13)	0.37204 (18)	0.8506 (4)	0.0151 (13)
C2	1.1602 (14)	0.33784 (19)	0.7534 (4)	0.0162 (13)

C3	1.2632 (16)	0.3281 (2)	0.6749 (4)	0.0236 (15)
H3	1.206730	0.342708	0.624462	0.028*
C4	1.4504 (15)	0.2966 (2)	0.6723 (4)	0.0261 (16)
H4	1.525655	0.289582	0.619464	0.031*
C5	1.5310 (15)	0.2748 (2)	0.7462 (5)	0.0262 (16)
H5	1.657929	0.253028	0.742875	0.031*
C6	1.4270 (15)	0.28477 (19)	0.8243 (4)	0.0201 (14)
H6	1.483893	0.270321	0.874871	0.024*
C7	1.2378 (14)	0.31638 (19)	0.8270 (4)	0.0168 (13)
S3	0.7312 (4)	0.42496 (5)	0.60016 (10)	0.0190 (3)
S4	0.3357 (4)	0.49495 (5)	0.57647 (10)	0.0180 (3)
N2	0.4180 (12)	0.45945 (16)	0.7190 (3)	0.0164 (12)
HN2	0.497 (15)	0.449 (2)	0.764 (3)	0.03 (2)*
C8	0.4996 (14)	0.45745 (19)	0.6383 (4)	0.0162 (13)
C9	0.2219 (14)	0.48927 (19)	0.7357 (4)	0.0174 (13)
C10	0.1004 (14)	0.4970 (2)	0.8131 (4)	0.0190 (14)
H10	0.149370	0.481541	0.862699	0.023*
C11	−0.0915 (15)	0.5276 (2)	0.8154 (4)	0.0221 (15)
H11	−0.179266	0.533075	0.867172	0.027*
C12	−0.1615 (15)	0.5510 (2)	0.7427 (4)	0.0208 (14)
H12	−0.295108	0.572001	0.746348	0.025*
C13	−0.0391 (14)	0.5439 (2)	0.6659 (4)	0.0220 (15)
H13	−0.083511	0.560008	0.617145	0.026*
C14	0.1515 (13)	0.51230 (19)	0.6627 (4)	0.0158 (13)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.0177 (2)	0.0159 (2)	0.01700 (19)	0.00011 (16)	0.00007 (16)	−0.00234 (17)
I2	0.0263 (2)	0.0245 (2)	0.0153 (2)	0.00547 (19)	−0.00254 (18)	−0.00115 (18)
I3	0.0171 (2)	0.0170 (2)	0.01558 (19)	0.00146 (16)	0.00089 (16)	−0.00224 (17)
I4	0.0313 (3)	0.0303 (3)	0.0169 (2)	0.0123 (2)	−0.00624 (19)	−0.00536 (19)
F1	0.032 (2)	0.019 (2)	0.0194 (19)	−0.0084 (17)	0.0019 (17)	0.0046 (17)
F2	0.028 (2)	0.029 (2)	0.027 (2)	−0.0075 (18)	−0.0056 (18)	−0.0054 (19)
F3	0.041 (3)	0.023 (2)	0.033 (2)	−0.0147 (19)	−0.001 (2)	0.0100 (19)
F4	0.040 (3)	0.025 (2)	0.0168 (19)	−0.0053 (19)	−0.0029 (18)	0.0056 (17)
F5	0.029 (2)	0.016 (2)	0.0167 (18)	−0.0053 (17)	0.0061 (16)	0.0037 (16)
F6	0.019 (2)	0.029 (2)	0.042 (3)	−0.0079 (18)	−0.0024 (19)	−0.010 (2)
F7	0.032 (2)	0.024 (2)	0.044 (3)	−0.0084 (19)	0.011 (2)	0.010 (2)
F8	0.029 (2)	0.028 (2)	0.0170 (19)	−0.0002 (18)	0.0002 (17)	0.0100 (17)
C15	0.010 (3)	0.016 (3)	0.019 (3)	0.000 (2)	0.002 (2)	−0.001 (3)
C16	0.017 (3)	0.013 (3)	0.020 (3)	0.001 (2)	0.005 (3)	0.003 (3)
C17	0.013 (3)	0.021 (4)	0.011 (3)	0.002 (3)	0.000 (2)	−0.001 (3)
C18	0.016 (3)	0.019 (4)	0.018 (3)	−0.002 (3)	−0.001 (3)	−0.002 (3)
C19	0.021 (4)	0.017 (4)	0.021 (3)	−0.004 (3)	0.004 (3)	−0.001 (3)
C20	0.024 (4)	0.017 (4)	0.014 (3)	0.004 (3)	0.001 (3)	0.001 (3)
C21	0.017 (3)	0.009 (3)	0.010 (3)	0.001 (2)	0.003 (2)	−0.001 (2)
C22	0.018 (3)	0.015 (3)	0.016 (3)	0.001 (3)	0.007 (3)	0.001 (3)

C23	0.017 (3)	0.016 (3)	0.016 (3)	0.004 (3)	−0.003 (3)	−0.002 (3)
C24	0.012 (3)	0.021 (4)	0.028 (4)	0.000 (3)	0.000 (3)	−0.008 (3)
C25	0.018 (3)	0.009 (3)	0.035 (4)	−0.002 (3)	0.007 (3)	0.006 (3)
C26	0.014 (3)	0.017 (3)	0.018 (3)	−0.001 (3)	0.004 (3)	0.002 (3)
I5	0.0251 (2)	0.0252 (3)	0.0291 (2)	0.00486 (19)	−0.00180 (19)	−0.0083 (2)
I6	0.0376 (3)	0.0383 (3)	0.0218 (2)	0.0001 (2)	0.0099 (2)	−0.0023 (2)
F13	0.037 (2)	0.029 (2)	0.024 (2)	0.002 (2)	0.0010 (19)	0.0053 (19)
F14	0.034 (3)	0.031 (3)	0.038 (2)	0.014 (2)	0.012 (2)	0.000 (2)
F15	0.047 (3)	0.033 (3)	0.032 (2)	0.005 (2)	−0.002 (2)	0.019 (2)
F16	0.036 (3)	0.045 (3)	0.021 (2)	0.009 (2)	0.0073 (19)	0.0024 (19)
C33	0.022 (4)	0.016 (3)	0.027 (4)	0.001 (3)	0.003 (3)	−0.004 (3)
C34	0.024 (4)	0.019 (4)	0.021 (3)	−0.005 (3)	−0.001 (3)	0.003 (3)
C35	0.024 (4)	0.021 (4)	0.021 (3)	−0.002 (3)	0.011 (3)	−0.003 (3)
C36	0.021 (4)	0.020 (4)	0.031 (4)	−0.001 (3)	0.002 (3)	−0.002 (3)
C37	0.023 (4)	0.030 (4)	0.028 (4)	0.001 (3)	0.006 (3)	0.008 (3)
C38	0.027 (4)	0.030 (4)	0.016 (3)	−0.001 (3)	0.006 (3)	0.002 (3)
I7	0.0204 (2)	0.0188 (2)	0.0290 (2)	−0.00085 (18)	−0.00007 (19)	−0.00546 (19)
I8	0.0220 (2)	0.0161 (2)	0.0263 (2)	−0.00127 (17)	0.00103 (18)	0.00192 (18)
F9	0.029 (2)	0.025 (2)	0.0171 (19)	−0.0009 (17)	−0.0005 (17)	−0.0004 (16)
F10	0.028 (2)	0.036 (3)	0.021 (2)	−0.0123 (19)	0.0001 (18)	−0.0051 (18)
F11	0.039 (3)	0.052 (3)	0.018 (2)	−0.013 (2)	0.0041 (19)	0.004 (2)
F12	0.026 (2)	0.030 (2)	0.034 (2)	−0.0084 (19)	0.0099 (19)	0.006 (2)
C27	0.015 (3)	0.009 (3)	0.025 (3)	−0.001 (2)	−0.002 (3)	−0.005 (3)
C28	0.018 (3)	0.016 (3)	0.015 (3)	0.003 (3)	0.001 (3)	0.002 (3)
C29	0.010 (3)	0.012 (3)	0.027 (3)	−0.001 (2)	0.004 (3)	−0.003 (3)
C30	0.018 (3)	0.027 (4)	0.021 (3)	−0.002 (3)	0.001 (3)	−0.005 (3)
C31	0.025 (4)	0.030 (4)	0.015 (3)	0.002 (3)	0.002 (3)	0.000 (3)
C32	0.017 (3)	0.016 (3)	0.030 (4)	0.000 (3)	0.010 (3)	0.000 (3)
S1	0.0189 (8)	0.0203 (9)	0.0175 (8)	0.0005 (7)	0.0009 (7)	−0.0035 (7)
S2	0.0224 (8)	0.0197 (9)	0.0134 (7)	−0.0011 (7)	−0.0004 (6)	0.0024 (6)
N1	0.022 (3)	0.014 (3)	0.010 (2)	0.000 (2)	0.000 (2)	0.002 (2)
C1	0.013 (3)	0.016 (3)	0.016 (3)	−0.004 (2)	0.000 (2)	−0.001 (3)
C2	0.015 (3)	0.017 (3)	0.016 (3)	−0.004 (3)	−0.002 (3)	−0.003 (3)
C3	0.024 (4)	0.030 (4)	0.016 (3)	0.001 (3)	0.002 (3)	0.001 (3)
C4	0.019 (4)	0.035 (4)	0.023 (4)	0.003 (3)	−0.003 (3)	−0.008 (3)
C5	0.017 (4)	0.027 (4)	0.033 (4)	0.004 (3)	−0.004 (3)	−0.008 (3)
C6	0.021 (4)	0.019 (4)	0.020 (3)	0.000 (3)	−0.003 (3)	−0.002 (3)
C7	0.016 (3)	0.018 (3)	0.015 (3)	−0.002 (3)	−0.004 (3)	−0.004 (3)
S3	0.0190 (8)	0.0206 (9)	0.0172 (8)	−0.0007 (7)	0.0001 (7)	−0.0018 (7)
S4	0.0191 (8)	0.0217 (9)	0.0129 (7)	−0.0017 (7)	0.0002 (6)	0.0016 (6)
N2	0.013 (3)	0.020 (3)	0.015 (3)	−0.001 (2)	−0.002 (2)	0.003 (2)
C8	0.017 (3)	0.018 (3)	0.013 (3)	−0.007 (3)	−0.001 (3)	−0.001 (2)
C9	0.017 (3)	0.019 (3)	0.015 (3)	−0.005 (3)	−0.004 (3)	−0.002 (3)
C10	0.021 (3)	0.022 (4)	0.014 (3)	−0.006 (3)	0.003 (3)	0.001 (3)
C11	0.026 (4)	0.025 (4)	0.016 (3)	−0.006 (3)	0.007 (3)	−0.008 (3)
C12	0.018 (3)	0.019 (4)	0.025 (4)	0.000 (3)	0.003 (3)	−0.006 (3)
C13	0.017 (3)	0.022 (4)	0.026 (4)	−0.003 (3)	−0.004 (3)	0.003 (3)
C14	0.011 (3)	0.020 (3)	0.015 (3)	−0.004 (3)	−0.002 (3)	−0.003 (3)

Geometric parameters (Å, º)

I1—C15	2.094 (6)	F11—C31	1.344 (7)
I2—C17	2.075 (6)	F12—C32	1.343 (7)
I3—C21	2.090 (6)	C27—C28	1.396 (9)
I4—C23	2.080 (6)	C27—C32	1.381 (9)
F1—C16	1.345 (7)	C28—C29	1.379 (9)
F2—C18	1.349 (8)	C29—C30	1.387 (9)
F3—C19	1.336 (7)	C30—C31	1.383 (9)
F4—C20	1.338 (7)	C31—C32	1.382 (10)
F5—C22	1.335 (7)	S1—C1	1.679 (6)
F6—C24	1.348 (8)	S2—C1	1.730 (7)
F7—C25	1.330 (7)	S2—C7	1.748 (7)
F8—C26	1.336 (7)	N1—HN1	0.89 (6)
C15—C16	1.386 (9)	N1—C1	1.347 (7)
C15—C20	1.389 (9)	N1—C2	1.401 (8)
C16—C17	1.391 (9)	C2—C3	1.389 (9)
C17—C18	1.381 (9)	C2—C7	1.385 (9)
C18—C19	1.383 (9)	C3—H3	0.9500
C19—C20	1.373 (10)	C3—C4	1.382 (10)
C21—C22	1.393 (8)	C4—H4	0.9500
C21—C26	1.387 (8)	C4—C5	1.398 (10)
C22—C23	1.389 (9)	C5—H5	0.9500
C23—C24	1.380 (10)	C5—C6	1.387 (9)
C24—C25	1.377 (10)	C6—H6	0.9500
C25—C26	1.384 (9)	C6—C7	1.390 (9)
I5—C33	2.080 (6)	S3—C8	1.679 (7)
I6—C35	2.073 (6)	S4—C8	1.741 (7)
F13—C34	1.351 (8)	S4—C14	1.748 (6)
F14—C36	1.346 (8)	N2—HN2	0.85 (3)
F15—C37	1.339 (8)	N2—C8	1.343 (8)
F16—C38	1.331 (7)	N2—C9	1.398 (8)
C33—C34	1.380 (9)	C9—C10	1.396 (9)
C33—C38	1.400 (10)	C9—C14	1.403 (9)
C34—C35	1.402 (9)	C10—H10	0.9500
C35—C36	1.373 (10)	C10—C11	1.369 (10)
C36—C37	1.375 (10)	C11—H11	0.9500
C37—C38	1.375 (10)	C11—C12	1.405 (9)
I7—C27	2.069 (6)	C12—H12	0.9500
I8—C29	2.085 (6)	C12—C13	1.384 (9)
F9—C28	1.342 (7)	C13—H13	0.9500
F10—C30	1.334 (8)	C13—C14	1.394 (9)
C16—C15—I1	122.6 (5)	C28—C29—C30	118.2 (6)
C16—C15—C20	117.1 (6)	C30—C29—I8	120.1 (5)
C20—C15—I1	120.2 (5)	F10—C30—C29	121.1 (6)
F1—C16—C15	118.3 (6)	F10—C30—C31	118.4 (6)
F1—C16—C17	118.4 (6)	C31—C30—C29	120.6 (6)

C15—C16—C17	123.2 (6)	F11—C31—C30	119.9 (6)
C16—C17—I2	121.1 (5)	F11—C31—C32	120.5 (6)
C18—C17—I2	121.8 (5)	C32—C31—C30	119.6 (6)
C18—C17—C16	117.1 (6)	F12—C32—C27	120.5 (6)
F2—C18—C17	120.3 (6)	F12—C32—C31	117.7 (6)
F2—C18—C19	118.0 (6)	C27—C32—C31	121.8 (6)
C17—C18—C19	121.7 (6)	C1—S2—C7	92.2 (3)
F3—C19—C18	120.4 (6)	C1—N1—HN1	117 (4)
F3—C19—C20	120.2 (6)	C1—N1—C2	115.5 (5)
C20—C19—C18	119.3 (6)	C2—N1—HN1	127 (4)
F4—C20—C15	120.0 (6)	S1—C1—S2	123.3 (4)
F4—C20—C19	118.3 (6)	N1—C1—S1	126.5 (5)
C19—C20—C15	121.6 (6)	N1—C1—S2	110.2 (5)
C22—C21—I3	122.5 (5)	C3—C2—N1	126.3 (6)
C26—C21—I3	120.1 (4)	C7—C2—N1	112.2 (6)
C26—C21—C22	117.3 (6)	C7—C2—C3	121.5 (6)
F5—C22—C21	118.4 (6)	C2—C3—H3	121.1
F5—C22—C23	118.9 (6)	C4—C3—C2	117.9 (6)
C23—C22—C21	122.7 (6)	C4—C3—H3	121.1
C22—C23—I4	120.7 (5)	C3—C4—H4	119.4
C24—C23—I4	122.0 (5)	C3—C4—C5	121.1 (7)
C24—C23—C22	117.3 (6)	C5—C4—H4	119.4
F6—C24—C23	120.0 (6)	C4—C5—H5	119.8
F6—C24—C25	117.8 (6)	C6—C5—C4	120.5 (7)
C25—C24—C23	122.2 (6)	C6—C5—H5	119.8
F7—C25—C24	120.7 (6)	C5—C6—H6	120.8
F7—C25—C26	120.3 (6)	C5—C6—C7	118.5 (6)
C24—C25—C26	118.9 (6)	C7—C6—H6	120.8
F8—C26—C21	120.4 (6)	C2—C7—S2	109.9 (5)
F8—C26—C25	117.9 (6)	C2—C7—C6	120.5 (6)
C25—C26—C21	121.6 (6)	C6—C7—S2	129.6 (5)
C34—C33—I5	121.5 (5)	C8—S4—C14	92.1 (3)
C34—C33—C38	117.3 (6)	C8—N2—HN2	129 (5)
C38—C33—I5	121.0 (5)	C8—N2—C9	116.3 (6)
F13—C34—C33	118.3 (6)	C9—N2—HN2	113 (5)
F13—C34—C35	118.6 (6)	S3—C8—S4	123.3 (4)
C33—C34—C35	123.1 (6)	N2—C8—S3	126.7 (5)
C34—C35—I6	121.7 (5)	N2—C8—S4	110.0 (5)
C36—C35—I6	121.7 (5)	N2—C9—C14	111.7 (6)
C36—C35—C34	116.6 (6)	C10—C9—N2	127.3 (6)
F14—C36—C35	119.6 (6)	C10—C9—C14	121.0 (6)
F14—C36—C37	117.8 (6)	C9—C10—H10	121.0
C35—C36—C37	122.6 (7)	C11—C10—C9	117.9 (6)
F15—C37—C36	120.0 (6)	C11—C10—H10	121.0
F15—C37—C38	120.8 (6)	C10—C11—H11	119.3
C38—C37—C36	119.2 (7)	C10—C11—C12	121.4 (6)
F16—C38—C33	119.7 (6)	C12—C11—H11	119.3
F16—C38—C37	119.1 (6)	C11—C12—H12	119.4

C37—C38—C33	121.2 (6)	C13—C12—C11	121.2 (6)
C28—C27—I7	121.9 (5)	C13—C12—H12	119.4
C32—C27—I7	121.2 (5)	C12—C13—H13	121.1
C32—C27—C28	116.9 (6)	C12—C13—C14	117.7 (6)
F9—C28—C27	118.2 (6)	C14—C13—H13	121.1
F9—C28—C29	118.9 (6)	C9—C14—S4	109.9 (5)
C29—C28—C27	122.9 (6)	C13—C14—S4	129.3 (5)
C28—C29—I8	121.6 (5)	C13—C14—C9	120.7 (6)

I1—C15—C16—F1	2.2 (8)	C35—C36—C37—C38	1.5 (11)
I1—C15—C16—C17	−176.3 (5)	C36—C37—C38—F16	179.3 (6)
I1—C15—C20—F4	−1.3 (8)	C36—C37—C38—C33	0.0 (11)
I1—C15—C20—C19	176.4 (5)	C38—C33—C34—F13	179.5 (6)
I2—C17—C18—F2	−0.2 (9)	C38—C33—C34—C35	0.1 (10)
I2—C17—C18—C19	−178.3 (5)	I7—C27—C28—F9	3.5 (8)
I3—C21—C22—F5	−2.7 (8)	I7—C27—C28—C29	−176.2 (5)
I3—C21—C22—C23	176.7 (5)	I7—C27—C32—F12	−4.9 (9)
I3—C21—C26—F8	1.3 (8)	I7—C27—C32—C31	174.8 (5)
I3—C21—C26—C25	−175.7 (5)	I8—C29—C30—F10	−3.5 (9)
I4—C23—C24—F6	−0.5 (9)	I8—C29—C30—C31	176.4 (5)
I4—C23—C24—C25	179.5 (5)	F9—C28—C29—I8	3.1 (8)
F1—C16—C17—I2	0.4 (8)	F9—C28—C29—C30	−179.0 (6)
F1—C16—C17—C18	−179.0 (6)	F10—C30—C31—F11	−0.2 (10)
F2—C18—C19—F3	−0.4 (10)	F10—C30—C31—C32	−179.9 (6)
F2—C18—C19—C20	−179.4 (6)	F11—C31—C32—F12	2.2 (10)
F3—C19—C20—F4	−0.8 (10)	F11—C31—C32—C27	−177.6 (6)
F3—C19—C20—C15	−178.5 (6)	C27—C28—C29—I8	−177.3 (5)
F5—C22—C23—I4	−0.1 (8)	C27—C28—C29—C30	0.6 (10)
F5—C22—C23—C24	177.8 (6)	C28—C27—C32—F12	177.4 (6)
F6—C24—C25—F7	2.8 (10)	C28—C27—C32—C31	−2.9 (10)
F6—C24—C25—C26	179.4 (6)	C28—C29—C30—F10	178.6 (6)
F7—C25—C26—F8	−1.0 (10)	C28—C29—C30—C31	−1.5 (10)
F7—C25—C26—C21	176.0 (6)	C29—C30—C31—F11	179.9 (6)
C15—C16—C17—I2	179.0 (5)	C29—C30—C31—C32	0.2 (10)
C15—C16—C17—C18	−0.4 (10)	C30—C31—C32—F12	−178.1 (6)
C16—C15—C20—F4	−177.5 (6)	C30—C31—C32—C27	2.1 (10)
C16—C15—C20—C19	0.2 (10)	C32—C27—C28—F9	−178.8 (6)
C16—C17—C18—F2	179.2 (6)	C32—C27—C28—C29	1.5 (10)
C16—C17—C18—C19	1.2 (10)	N1—C2—C3—C4	−179.8 (6)
C17—C18—C19—F3	177.7 (6)	N1—C2—C7—S2	−0.7 (7)
C17—C18—C19—C20	−1.3 (11)	N1—C2—C7—C6	−179.7 (6)
C18—C19—C20—F4	178.3 (6)	C1—S2—C7—C2	0.5 (5)
C18—C19—C20—C15	0.6 (10)	C1—S2—C7—C6	179.4 (7)
C20—C15—C16—F1	178.3 (5)	C1—N1—C2—C3	179.5 (6)
C20—C15—C16—C17	−0.2 (10)	C1—N1—C2—C7	0.6 (8)
C21—C22—C23—I4	−179.5 (5)	C2—N1—C1—S1	−179.8 (5)
C21—C22—C23—C24	−1.5 (10)	C2—N1—C1—S2	−0.2 (7)
C22—C21—C26—F8	177.6 (6)	C2—C3—C4—C5	0.8 (11)

C22—C21—C26—C25	0.7 (9)	C3—C2—C7—S2	−179.7 (5)
C22—C23—C24—F6	−178.3 (6)	C3—C2—C7—C6	1.3 (10)
C22—C23—C24—C25	1.6 (10)	C3—C4—C5—C6	−0.8 (11)
C23—C24—C25—F7	−177.2 (6)	C4—C5—C6—C7	1.1 (10)
C23—C24—C25—C26	−0.6 (10)	C5—C6—C7—S2	179.9 (5)
C24—C25—C26—F8	−177.7 (6)	C5—C6—C7—C2	−1.3 (10)
C24—C25—C26—C21	−0.6 (10)	C7—S2—C1—S1	179.5 (4)
C26—C21—C22—F5	−178.9 (5)	C7—S2—C1—N1	−0.2 (5)
C26—C21—C22—C23	0.4 (9)	C7—C2—C3—C4	−1.0 (10)
I5—C33—C34—F13	4.8 (9)	N2—C9—C10—C11	−179.2 (6)
I5—C33—C34—C35	−174.6 (5)	N2—C9—C14—S4	0.3 (7)
I5—C33—C38—F16	−5.4 (9)	N2—C9—C14—C13	−179.4 (6)
I5—C33—C38—C37	174.0 (6)	C8—S4—C14—C9	0.4 (5)
I6—C35—C36—F14	−1.7 (10)	C8—S4—C14—C13	−180.0 (6)
I6—C35—C36—C37	178.9 (6)	C8—N2—C9—C10	178.6 (6)
F13—C34—C35—I6	0.9 (9)	C8—N2—C9—C14	−1.1 (8)
F13—C34—C35—C36	−178.2 (6)	C9—N2—C8—S3	179.9 (5)
F14—C36—C37—F15	1.1 (10)	C9—N2—C8—S4	1.4 (7)
F14—C36—C37—C38	−177.9 (7)	C9—C10—C11—C12	−1.0 (10)
F15—C37—C38—F16	0.4 (11)	C10—C9—C14—S4	−179.5 (5)
F15—C37—C38—C33	−179.0 (7)	C10—C9—C14—C13	0.8 (10)
C33—C34—C35—I6	−179.8 (5)	C10—C11—C12—C13	0.2 (11)
C33—C34—C35—C36	1.2 (10)	C11—C12—C13—C14	1.2 (10)
C34—C33—C38—F16	179.9 (6)	C12—C13—C14—S4	178.7 (5)
C34—C33—C38—C37	−0.8 (11)	C12—C13—C14—C9	−1.7 (10)
C34—C35—C36—F14	177.3 (6)	C14—S4—C8—S3	−179.6 (4)
C34—C35—C36—C37	−2.0 (11)	C14—S4—C8—N2	−1.0 (5)
C35—C36—C37—F15	−179.5 (7)	C14—C9—C10—C11	0.5 (10)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···S3	0.89 (6)	2.51 (6)	3.376 (6)	165 (5)
C3—H3···I1	0.95	3.10	3.976 (7)	154
N2—H*N*2···S1	0.85 (3)	2.52 (3)	3.360 (6)	169 (7)
C10—H10···I3^{i}	0.95	3.09	4.006 (6)	161

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

1,3-Benzothiazole-2-thiol–1,2,4,5-tetrafluoro-3,6-diiodobenzene (2/1) (2MBZTH_14F4DIB)

Crystal data

$C_6F_4I_2·2C_7H_5NS_2$
M_r = 736.34
Monoclinic, $P2_1/n$
a = 5.5057 (2) Å
b = 15.6087 (7) Å
c = 13.5194 (6) Å
β = 94.259 (2)°
V = 1158.61 (8) Å^3
Z = 2
F(000) = 700
D_x = 2.111 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9937 reflections
θ = 2.6–30.1°

μ = 3.12 mm^{-1}
T = 100 K

Needle, colourless
0.17 × 0.09 × 0.04 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec IμS
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.559, T_{max} = 0.746
22270 measured reflections

3402 independent reflections
2811 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 30.1°, θ_{min} = 2.6°
h = −7→7
k = −22→21
l = −18→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.057
S = 1.15
3402 reflections
149 parameters
0 restraints
Primary atom site location: dual

Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0092P)^2 + 1.689P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.90 e Å^{-3}
$\Delta\rho_{min}$ = −0.78 e Å^{-3}

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.

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

	x	y	z	U_{iso}*/U_{eq}
I1	0.09620 (3)	0.50667 (2)	0.18841 (2)	0.01843 (6)
F1	0.4987 (3)	0.36936 (10)	0.13226 (14)	0.0285 (4)
F2	0.8063 (3)	0.36478 (10)	−0.00971 (13)	0.0267 (4)
C8	0.3371 (5)	0.50280 (17)	0.0761 (2)	0.0179 (5)
C9	0.4956 (5)	0.43488 (17)	0.0673 (2)	0.0210 (6)
C10	0.6546 (5)	0.43202 (17)	−0.0070 (2)	0.0190 (5)
S1	−0.29400 (12)	0.50758 (4)	0.36239 (5)	0.01927 (14)
S2	0.07419 (13)	0.64355 (4)	0.42496 (5)	0.02067 (15)
N1	−0.2698 (4)	0.60239 (14)	0.52996 (18)	0.0175 (5)
HN1	−0.379 (6)	0.577 (2)	0.548 (3)	0.024 (9)*
C1	−0.1812 (5)	0.58112 (16)	0.4433 (2)	0.0166 (5)
C2	−0.1450 (5)	0.66593 (16)	0.5855 (2)	0.0173 (5)
C3	−0.2004 (5)	0.69814 (17)	0.6767 (2)	0.0225 (6)
H3	−0.337581	0.678027	0.708502	0.027*
C4	−0.0491 (6)	0.76050 (19)	0.7197 (2)	0.0271 (7)
H4	−0.083090	0.783531	0.782261	0.032*
C5	0.1516 (6)	0.79028 (19)	0.6737 (2)	0.0269 (7)
H5	0.253410	0.832708	0.705534	0.032*
C6	0.2060 (5)	0.75900 (17)	0.5816 (2)	0.0237 (6)

H6	0.342177	0.779762	0.549629	0.028*
C7	0.0542 (5)	0.69629 (16)	0.5379 (2)	0.0178 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01632 (9)	0.02275 (9)	0.01671 (10)	0.00025 (7)	0.00446 (6)	−0.00296 (6)
F1	0.0349 (10)	0.0250 (8)	0.0273 (10)	0.0077 (7)	0.0135 (8)	0.0069 (7)
F2	0.0284 (9)	0.0247 (8)	0.0283 (10)	0.0099 (7)	0.0107 (8)	0.0003 (7)
C8	0.0152 (12)	0.0226 (13)	0.0162 (14)	−0.0007 (10)	0.0035 (10)	−0.0063 (10)
C9	0.0216 (14)	0.0217 (13)	0.0200 (15)	−0.0003 (11)	0.0031 (12)	−0.0003 (10)
C10	0.0169 (12)	0.0196 (12)	0.0207 (15)	0.0022 (10)	0.0019 (11)	−0.0047 (10)
S1	0.0194 (3)	0.0228 (3)	0.0161 (3)	−0.0054 (3)	0.0047 (3)	−0.0013 (2)
S2	0.0195 (3)	0.0236 (3)	0.0198 (4)	−0.0062 (3)	0.0071 (3)	−0.0005 (3)
N1	0.0170 (11)	0.0165 (10)	0.0196 (13)	−0.0033 (9)	0.0057 (9)	0.0011 (9)
C1	0.0154 (12)	0.0176 (12)	0.0170 (14)	−0.0002 (10)	0.0030 (10)	0.0036 (9)
C2	0.0189 (13)	0.0148 (11)	0.0184 (14)	−0.0022 (10)	0.0016 (11)	0.0020 (9)
C3	0.0227 (14)	0.0226 (13)	0.0230 (16)	0.0016 (11)	0.0061 (12)	0.0009 (11)
C4	0.0322 (16)	0.0254 (14)	0.0238 (17)	0.0003 (12)	0.0036 (13)	−0.0066 (12)
C5	0.0273 (15)	0.0221 (14)	0.0307 (18)	−0.0041 (12)	−0.0022 (13)	−0.0029 (12)
C6	0.0232 (14)	0.0194 (13)	0.0286 (17)	−0.0051 (11)	0.0023 (12)	0.0013 (11)
C7	0.0173 (12)	0.0170 (12)	0.0193 (15)	−0.0007 (10)	0.0027 (11)	0.0026 (10)

Geometric parameters (Å, º)

I1—C8	2.090 (3)	N1—C2	1.394 (4)
F1—C9	1.348 (3)	C2—C3	1.386 (4)
F2—C10	1.344 (3)	C2—C7	1.395 (4)
C8—C9	1.384 (4)	C3—H3	0.9500
C8—C10^{i}	1.385 (4)	C3—C4	1.381 (4)
C9—C10	1.381 (4)	C4—H4	0.9500
S1—C1	1.673 (3)	C4—C5	1.388 (4)
S2—C1	1.743 (3)	C5—H5	0.9500
S2—C7	1.746 (3)	C5—C6	1.390 (4)
N1—HN1	0.78 (3)	C6—H6	0.9500
N1—C1	1.344 (3)	C6—C7	1.390 (4)
C9—C8—I1	121.6 (2)	C3—C2—N1	127.2 (2)
C9—C8—C10^{i}	116.8 (2)	C3—C2—C7	121.3 (3)
C10^{i}—C8—I1	121.59 (19)	C2—C3—H3	121.2
F1—C9—C8	120.2 (2)	C4—C3—C2	117.7 (3)
F1—C9—C10	118.1 (2)	C4—C3—H3	121.2
C10—C9—C8	121.7 (3)	C3—C4—H4	119.3
F2—C10—C8^{i}	120.2 (2)	C3—C4—C5	121.5 (3)
F2—C10—C9	118.3 (2)	C5—C4—H4	119.3
C9—C10—C8^{i}	121.4 (2)	C4—C5—H5	119.5
C1—S2—C7	92.03 (13)	C4—C5—C6	121.0 (3)
C1—N1—HN1	119 (3)	C6—C5—H5	119.5

C1—N1—C2	116.7 (2)	C5—C6—H6	121.1
C2—N1—HN1	124 (3)	C7—C6—C5	117.7 (3)
S1—C1—S2	123.72 (16)	C7—C6—H6	121.1
N1—C1—S1	126.7 (2)	C2—C7—S2	110.2 (2)
N1—C1—S2	109.5 (2)	C6—C7—S2	128.9 (2)
N1—C2—C7	111.5 (2)	C6—C7—C2	120.8 (3)
I1—C8—C9—F1	−0.5 (4)	C1—N1—C2—C7	0.3 (3)
I1—C8—C9—C10	179.8 (2)	C2—N1—C1—S1	−180.0 (2)
F1—C9—C10—F2	−0.9 (4)	C2—N1—C1—S2	−0.7 (3)
F1—C9—C10—C8^{i}	−179.6 (3)	C2—C3—C4—C5	0.1 (5)
C8—C9—C10—F2	178.7 (3)	C3—C2—C7—S2	−179.8 (2)
C8—C9—C10—C8^{i}	0.0 (5)	C3—C2—C7—C6	1.1 (4)
C10^{i}—C8—C9—F1	179.6 (3)	C3—C4—C5—C6	0.8 (5)
C10^{i}—C8—C9—C10	0.0 (5)	C4—C5—C6—C7	−0.7 (5)
N1—C2—C3—C4	179.0 (3)	C5—C6—C7—S2	−179.2 (2)
N1—C2—C7—S2	0.2 (3)	C5—C6—C7—C2	−0.2 (4)
N1—C2—C7—C6	−178.9 (3)	C7—S2—C1—S1	180.00 (19)
C1—S2—C7—C2	−0.5 (2)	C7—S2—C1—N1	0.7 (2)
C1—S2—C7—C6	178.5 (3)	C7—C2—C3—C4	−1.0 (4)
C1—N1—C2—C3	−179.7 (3)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···S1^{ii}	0.78 (3)	2.60 (3)	3.369 (2)	170 (3)
C3—H3···F1^{iii}	0.95	2.50	3.333 (3)	146
C6—H6···F2^{iv}	0.95	2.44	3.357 (3)	162

Symmetry codes: (ii) −*x*−1, −*y*+1, −*z*+1; (iii) −*x*, −*y*+1, −*z*+1; (iv) −*x*+3/2, *y*+1/2, −*z*+1/2.

1,3-Benzothiazole-2-thiol–1,3,5-trifluoro-2,4,6-triiodobenzene (1/1) (MBZTH_135F3I3B)

Crystal data

$C_6F_3I_3·C_7H_5NS_2$
M_r = 677.00
Monoclinic, $P2_1/c$
a = 15.2665 (6) Å
b = 4.7380 (2) Å
c = 23.2215 (10) Å
β = 93.139 (2)°
V = 1677.15 (12) Å^3
Z = 4
$F(000)$ = 1232
D_x = 2.681 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9894 reflections
θ = 3.1–28.4°
μ = 5.86 mm^{-1}
T = 100 K
Plate, colourless
0.16 × 0.08 × 0.05 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec IμS
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
T_{min} = 0.610, T_{max} = 0.746
35222 measured reflections
4212 independent reflections

3611 reflections with $I > 2\sigma(I)$
$R_{int} = 0.057$
$\theta_{max} = 28.4°$, $\theta_{min} = 2.2°$
$h = -19 \rightarrow 20$
$k = -6 \rightarrow 6$
$l = -30 \rightarrow 31$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.024$
$wR(F^2) = 0.052$
$S = 1.18$
4212 reflections
203 parameters
1 restraint
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + 4.0997P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 0.67$ e Å^{-3}
$\Delta\rho_{min} = -0.73$ e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.70161 (2)	0.58105 (5)	0.55847 (2)	0.01897 (6)
I2	0.68104 (2)	−0.18871 (6)	0.76567 (2)	0.02456 (7)
I3	0.37648 (2)	−0.11384 (6)	0.58903 (2)	0.02243 (6)
F1	0.75133 (13)	0.2505 (5)	0.67513 (9)	0.0224 (5)
F2	0.49679 (14)	−0.2816 (5)	0.70076 (9)	0.0247 (5)
F3	0.51145 (13)	0.3138 (5)	0.54048 (9)	0.0224 (5)
C8	0.6317 (2)	0.2972 (7)	0.60769 (15)	0.0161 (7)
C9	0.6683 (2)	0.1805 (8)	0.65793 (15)	0.0168 (7)
C10	0.6242 (2)	−0.0129 (8)	0.69039 (15)	0.0170 (7)
C11	0.5404 (2)	−0.0910 (8)	0.67047 (15)	0.0195 (7)
C12	0.5008 (2)	0.0172 (8)	0.62016 (15)	0.0170 (7)
C13	0.5477 (2)	0.2102 (8)	0.58980 (15)	0.0177 (7)
S1	0.85079 (6)	1.0132 (2)	0.49475 (4)	0.02217 (19)
S2	0.81182 (6)	0.6044 (2)	0.39819 (4)	0.02095 (19)
N1	0.9677 (2)	0.7071 (7)	0.43672 (13)	0.0205 (6)
HN1	1.011 (2)	0.777 (10)	0.4571 (18)	0.040 (14)*
C1	0.8842 (2)	0.7835 (8)	0.44595 (15)	0.0185 (7)
C2	0.9777 (2)	0.5076 (8)	0.39362 (16)	0.0203 (7)
C3	1.0556 (3)	0.3935 (9)	0.37636 (18)	0.0278 (9)
H3	1.110354	0.453291	0.393589	0.033*
C4	1.0518 (3)	0.1913 (9)	0.33364 (18)	0.0303 (9)
H4	1.104619	0.107792	0.322010	0.036*
C5	0.9720 (3)	0.1072 (9)	0.30721 (18)	0.0304 (9)
H5	0.971216	−0.031349	0.277614	0.036*
C6	0.8934 (3)	0.2228 (8)	0.32348 (17)	0.0260 (8)
H6	0.838874	0.165478	0.305463	0.031*
C7	0.8970 (2)	0.4256 (8)	0.36705 (15)	0.0194 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01882 (12)	0.01952 (12)	0.01885 (12)	−0.00162 (9)	0.00346 (9)	−0.00136 (9)
I2	0.02741 (13)	0.02835 (14)	0.01735 (12)	0.00846 (10)	−0.00403 (9)	0.00139 (10)
I3	0.01542 (11)	0.03132 (14)	0.02042 (12)	−0.00464 (9)	−0.00022 (9)	−0.00501 (10)
F1	0.0151 (10)	0.0285 (12)	0.0230 (11)	−0.0008 (9)	−0.0039 (8)	−0.0038 (9)
F2	0.0261 (11)	0.0259 (12)	0.0221 (11)	−0.0066 (9)	0.0014 (9)	0.0078 (9)
F3	0.0198 (10)	0.0286 (12)	0.0184 (10)	0.0021 (9)	−0.0027 (8)	0.0066 (9)
C8	0.0174 (16)	0.0146 (17)	0.0163 (16)	−0.0009 (13)	0.0025 (13)	−0.0019 (13)
C9	0.0137 (16)	0.0191 (17)	0.0175 (17)	0.0018 (13)	−0.0010 (13)	−0.0058 (14)
C10	0.0180 (17)	0.0184 (17)	0.0142 (16)	0.0044 (13)	−0.0036 (13)	−0.0014 (14)
C11	0.0206 (18)	0.0202 (18)	0.0180 (17)	−0.0001 (14)	0.0032 (14)	−0.0004 (14)
C12	0.0130 (16)	0.0198 (18)	0.0180 (17)	−0.0001 (13)	0.0000 (13)	−0.0020 (14)
C13	0.0159 (16)	0.0208 (18)	0.0163 (16)	0.0037 (14)	0.0007 (13)	−0.0005 (14)
S1	0.0217 (5)	0.0233 (5)	0.0217 (5)	−0.0019 (4)	0.0019 (4)	−0.0025 (4)
S2	0.0158 (4)	0.0237 (5)	0.0229 (5)	−0.0027 (3)	−0.0021 (3)	−0.0020 (4)
N1	0.0183 (15)	0.0251 (17)	0.0178 (15)	−0.0035 (13)	−0.0019 (12)	−0.0011 (13)
C1	0.0178 (17)	0.0183 (18)	0.0191 (17)	−0.0026 (14)	−0.0004 (14)	0.0025 (14)
C2	0.0218 (18)	0.0196 (18)	0.0194 (18)	0.0014 (14)	−0.0019 (14)	0.0022 (15)
C3	0.0201 (19)	0.033 (2)	0.030 (2)	0.0003 (16)	−0.0023 (16)	0.0032 (18)
C4	0.033 (2)	0.031 (2)	0.028 (2)	0.0097 (18)	0.0072 (17)	0.0002 (18)
C5	0.043 (3)	0.022 (2)	0.026 (2)	0.0013 (18)	0.0067 (18)	−0.0007 (17)
C6	0.033 (2)	0.022 (2)	0.0223 (19)	−0.0059 (16)	−0.0037 (16)	0.0010 (16)
C7	0.0198 (18)	0.0199 (18)	0.0183 (17)	−0.0008 (14)	0.0004 (14)	0.0026 (14)

Geometric parameters (Å, º)

I1—C8	2.095 (3)	S2—C7	1.742 (4)
I2—C10	2.082 (3)	N1—HN1	0.857 (19)
I3—C12	2.088 (3)	N1—C1	1.353 (5)
F1—C9	1.349 (4)	N1—C2	1.391 (5)
F2—C11	1.343 (4)	C2—C3	1.386 (5)
F3—C13	1.338 (4)	C2—C7	1.402 (5)
C8—C9	1.381 (5)	C3—H3	0.9500
C8—C13	1.389 (5)	C3—C4	1.378 (6)
C9—C10	1.384 (5)	C4—H4	0.9500
C10—C11	1.388 (5)	C4—C5	1.393 (6)
C11—C12	1.384 (5)	C5—H5	0.9500
C12—C13	1.379 (5)	C5—C6	1.390 (6)
S1—C1	1.671 (4)	C6—H6	0.9500
S2—C1	1.743 (4)	C6—C7	1.394 (5)
C9—C8—I1	121.6 (3)	S1—C1—S2	122.8 (2)
C9—C8—C13	117.3 (3)	N1—C1—S1	127.4 (3)
C13—C8—I1	121.1 (3)	N1—C1—S2	109.8 (3)
F1—C9—C8	118.8 (3)	N1—C2—C7	112.1 (3)
F1—C9—C10	118.6 (3)	C3—C2—N1	127.1 (4)

C8—C9—C10	122.6 (3)	C3—C2—C7	120.8 (4)
C9—C10—I2	122.0 (3)	C2—C3—H3	120.8
C9—C10—C11	117.5 (3)	C4—C3—C2	118.5 (4)
C11—C10—I2	120.5 (3)	C4—C3—H3	120.8
F2—C11—C10	118.6 (3)	C3—C4—H4	119.4
F2—C11—C12	119.0 (3)	C3—C4—C5	121.1 (4)
C12—C11—C10	122.3 (3)	C5—C4—H4	119.4
C11—C12—I3	121.9 (3)	C4—C5—H5	119.5
C13—C12—I3	120.5 (3)	C6—C5—C4	121.0 (4)
C13—C12—C11	117.6 (3)	C6—C5—H5	119.5
F3—C13—C8	118.7 (3)	C5—C6—H6	121.0
F3—C13—C12	118.6 (3)	C5—C6—C7	117.9 (4)
C12—C13—C8	122.7 (3)	C7—C6—H6	121.0
C7—S2—C1	92.24 (18)	C2—C7—S2	109.9 (3)
C1—N1—HN1	121 (3)	C6—C7—S2	129.5 (3)
C1—N1—C2	115.9 (3)	C6—C7—C2	120.6 (3)
C2—N1—HN1	123 (3)		

I1—C8—C9—F1	−0.5 (4)	C13—C8—C9—F1	177.0 (3)
I1—C8—C9—C10	−178.3 (3)	C13—C8—C9—C10	−0.8 (5)
I1—C8—C13—F3	−0.7 (4)	N1—C2—C3—C4	178.2 (4)
I1—C8—C13—C12	178.0 (3)	N1—C2—C7—S2	−0.2 (4)
I2—C10—C11—F2	0.1 (5)	N1—C2—C7—C6	−178.7 (3)
I2—C10—C11—C12	−178.9 (3)	C1—S2—C7—C2	−0.2 (3)
I3—C12—C13—F3	0.8 (5)	C1—S2—C7—C6	178.1 (4)
I3—C12—C13—C8	−177.9 (3)	C1—N1—C2—C3	−179.4 (4)
F1—C9—C10—I2	1.7 (4)	C1—N1—C2—C7	0.8 (5)
F1—C9—C10—C11	−177.2 (3)	C2—N1—C1—S1	179.2 (3)
F2—C11—C12—I3	−1.4 (5)	C2—N1—C1—S2	−0.9 (4)
F2—C11—C12—C13	−179.3 (3)	C2—C3—C4—C5	1.5 (6)
C8—C9—C10—I2	179.5 (3)	C3—C2—C7—S2	179.9 (3)
C8—C9—C10—C11	0.6 (5)	C3—C2—C7—C6	1.4 (6)
C9—C8—C13—F3	−178.2 (3)	C3—C4—C5—C6	−0.6 (6)
C9—C8—C13—C12	0.4 (5)	C4—C5—C6—C7	0.0 (6)
C9—C10—C11—F2	179.0 (3)	C5—C6—C7—S2	−178.6 (3)
C9—C10—C11—C12	0.0 (5)	C5—C6—C7—C2	−0.4 (6)
C10—C11—C12—I3	177.6 (3)	C7—S2—C1—S1	−179.5 (2)
C10—C11—C12—C13	−0.4 (5)	C7—S2—C1—N1	0.6 (3)
C11—C12—C13—F3	178.8 (3)	C7—C2—C3—C4	−1.9 (6)
C11—C12—C13—C8	0.1 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···S1^{i}	0.86 (2)	2.54 (2)	3.389 (3)	172 (4)
C3—H3···I1^{ii}	0.95	3.03	3.928 (4)	159

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

1,3-Benzothiazole-2-thiol–1,1,2,2-tetraiodoethene (1/1) (MBZTH_TIE)

Crystal data

$C_2I_4 \cdot C_7H_5NS_2$
$M_r = 698.86$
Triclinic, $P\overline{1}$
$a = 7.4085$ (6) Å
$b = 10.8180$ (9) Å
$c = 11.1989$ (10) Å
$\alpha = 66.616$ (3)°
$\beta = 70.765$ (3)°
$\gamma = 70.792$ (3)°
$V = 757.20$ (11) Å^3
$Z = 2$
$F(000) = 620$
$D_x = 3.065$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9908 reflections
$\theta = 2.4$–$27.6°$
$\mu = 8.48$ mm^{-1}
$T = 100$ K
Block, yellow
0.08 × 0.07 × 0.07 mm

Data collection

Bruker D8 Venture Photon 2 diffractometer
Radiation source: Incoatec IμS
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2017)
$T_{min} = 0.589$, $T_{max} = 0.746$
22463 measured reflections
3484 independent reflections
3037 reflections with $I > 2\sigma(I)$
$R_{int} = 0.052$
$\theta_{max} = 27.6°$, $\theta_{min} = 2.1°$
$h = -9 \rightarrow 9$
$k = -14 \rightarrow 14$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.072$
$S = 1.13$
3484 reflections
159 parameters
7 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0264P)^2 + 3.2353P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 1.43$ e Å^{-3}
$\Delta\rho_{min} = -1.76$ e Å^{-3}

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.

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

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
I1	0.18703 (5)	0.90012 (3)	0.68231 (3)	0.02172 (9)	
I2	0.32280 (5)	0.95731 (4)	0.33480 (3)	0.02290 (9)	
C8	0.0936 (8)	0.9743 (5)	0.5033 (6)	0.0239 (11)	
I3	0.72172 (6)	0.21253 (4)	0.95745 (4)	0.03285 (11)	
I4	0.76779 (5)	−0.15110 (4)	1.05340 (4)	0.02545 (10)	
C9A	0.9080 (15)	0.0083 (10)	1.0028 (9)	0.016 (3)	0.529 (19)
C9B	0.9990 (16)	−0.0669 (12)	1.0232 (11)	0.016 (3)	0.471 (19)
S1	0.33205 (18)	0.46883 (15)	0.92558 (14)	0.0257 (3)	
S2	0.34982 (18)	0.53599 (14)	0.63493 (13)	0.0224 (3)	

N1	0.0271 (6)	0.5607 (5)	0.8065 (4)	0.0207 (9)
HN1	−0.057 (8)	0.555 (7)	0.881 (4)	0.036 (19)*
C1	0.2213 (7)	0.5214 (5)	0.7989 (5)	0.0193 (10)
C2	0.1323 (7)	0.6027 (5)	0.5783 (5)	0.0189 (10)
C3	0.1076 (8)	0.6481 (6)	0.4478 (6)	0.0245 (11)
H3	0.217056	0.642904	0.374510	0.029*
C4	−0.0808 (9)	0.7004 (6)	0.4295 (6)	0.0270 (12)
H4	−0.101730	0.733475	0.341722	0.032*
C5	−0.2416 (8)	0.7059 (6)	0.5370 (6)	0.0272 (12)
H5	−0.369991	0.742518	0.520859	0.033*
C6	−0.2192 (8)	0.6593 (5)	0.6671 (6)	0.0233 (11)
H6	−0.329217	0.662174	0.740411	0.028*
C7	−0.0280 (7)	0.6081 (5)	0.6852 (5)	0.0187 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01984 (17)	0.02418 (18)	0.02146 (18)	−0.00095 (13)	−0.00713 (13)	−0.00908 (13)
I2	0.01628 (16)	0.02862 (19)	0.02166 (18)	−0.00312 (13)	−0.00118 (13)	−0.01016 (14)
C8	0.024 (3)	0.020 (2)	0.025 (3)	0.002 (2)	−0.006 (2)	−0.009 (2)
I3	0.0351 (2)	0.0308 (2)	0.0316 (2)	0.01363 (16)	−0.01664 (17)	−0.01885 (16)
I4	0.02582 (18)	0.02565 (18)	0.02593 (19)	−0.01160 (14)	−0.00886 (14)	−0.00245 (14)
C9A	0.020 (5)	0.005 (4)	0.016 (4)	0.003 (4)	−0.004 (3)	−0.001 (3)
C9B	0.009 (5)	0.012 (6)	0.019 (5)	0.003 (4)	−0.004 (4)	−0.003 (4)
S1	0.0144 (6)	0.0329 (7)	0.0213 (6)	0.0021 (5)	−0.0034 (5)	−0.0067 (6)
S2	0.0158 (6)	0.0261 (6)	0.0215 (6)	−0.0002 (5)	−0.0008 (5)	−0.0105 (5)
N1	0.017 (2)	0.021 (2)	0.019 (2)	−0.0026 (17)	−0.0031 (17)	−0.0042 (18)
C1	0.016 (2)	0.015 (2)	0.024 (3)	−0.0034 (18)	−0.004 (2)	−0.005 (2)
C2	0.017 (2)	0.018 (2)	0.022 (3)	−0.0040 (19)	−0.0020 (19)	−0.008 (2)
C3	0.026 (3)	0.026 (3)	0.022 (3)	−0.005 (2)	−0.002 (2)	−0.012 (2)
C4	0.031 (3)	0.024 (3)	0.025 (3)	−0.009 (2)	−0.005 (2)	−0.005 (2)
C5	0.025 (3)	0.021 (3)	0.034 (3)	0.000 (2)	−0.012 (2)	−0.006 (2)
C6	0.019 (2)	0.020 (2)	0.029 (3)	−0.002 (2)	−0.004 (2)	−0.008 (2)
C7	0.020 (2)	0.015 (2)	0.018 (2)	−0.0022 (18)	−0.002 (2)	−0.0051 (19)

Geometric parameters (Å, º)

I1—C8	2.101 (6)	N1—C1	1.343 (6)
I2—C8	2.106 (6)	N1—C7	1.396 (7)
C8—C8^{i}	1.329 (11)	C2—C3	1.400 (8)
I3—C9A	2.146 (10)	C2—C7	1.386 (7)
I3—C9B^{ii}	2.166 (11)	C3—H3	0.9500
I4—C9A	2.095 (10)	C3—C4	1.373 (8)
I4—C9B	2.069 (11)	C4—H4	0.9500
C9A—C9A^{ii}	1.30 (2)	C4—C5	1.392 (8)
C9B—C9B^{ii}	1.33 (2)	C5—H5	0.9500
S1—C1	1.682 (5)	C5—C6	1.388 (8)
S2—C1	1.738 (5)	C6—H6	0.9500

S2—C2	1.750 (5)	C6—C7	1.392 (7)
N1—HN1	0.85 (2)		
I1—C8—I2	114.1 (2)	C7—C2—S2	109.9 (4)
C8^{i}—C8—I1	123.2 (6)	C7—C2—C3	121.0 (5)
C8^{i}—C8—I2	122.8 (6)	C2—C3—H3	121.2
C9A—I3—C9B^{ii}	26.4 (4)	C4—C3—C2	117.6 (5)
I4—C9A—I3	114.6 (5)	C4—C3—H3	121.2
C9A^{ii}—C9A—I3	120.0 (10)	C3—C4—H4	119.4
C9A^{ii}—C9A—I4	125.3 (10)	C3—C4—C5	121.3 (6)
I4—C9B—I3^{ii}	115.8 (5)	C5—C4—H4	119.4
C9B^{ii}—C9B—I4	127.1 (11)	C4—C5—H5	119.2
C1—S2—C2	91.8 (2)	C6—C5—C4	121.7 (5)
C1—N1—HN1	122 (5)	C6—C5—H5	119.2
C1—N1—C7	115.7 (4)	C5—C6—H6	121.5
C7—N1—HN1	122 (5)	C5—C6—C7	116.9 (5)
S1—C1—S2	123.1 (3)	C7—C6—H6	121.5
N1—C1—S1	126.6 (4)	C2—C7—N1	112.4 (4)
N1—C1—S2	110.2 (4)	C2—C7—C6	121.5 (5)
C3—C2—S2	129.1 (4)	C6—C7—N1	126.1 (5)
S2—C2—C3—C4	−178.0 (4)	C3—C2—C7—N1	−178.9 (5)
S2—C2—C7—N1	0.4 (5)	C3—C2—C7—C6	−0.3 (8)
S2—C2—C7—C6	179.0 (4)	C3—C4—C5—C6	0.2 (9)
C1—S2—C2—C3	177.8 (5)	C4—C5—C6—C7	0.7 (8)
C1—S2—C2—C7	−1.4 (4)	C5—C6—C7—N1	177.7 (5)
C1—N1—C7—C2	1.3 (6)	C5—C6—C7—C2	−0.7 (8)
C1—N1—C7—C6	−177.3 (5)	C7—N1—C1—S1	176.2 (4)
C2—S2—C1—S1	−176.4 (3)	C7—N1—C1—S2	−2.3 (6)
C2—S2—C1—N1	2.1 (4)	C7—C2—C3—C4	1.2 (8)
C2—C3—C4—C5	−1.1 (8)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H*N*1···S1^{iii}	0.85 (2)	2.43 (2)	3.275 (5)	170 (6)

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