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4-Amino-3-[2-(9*H*-carbazol-9-yl)ethyl]-1*H*-1,2,4-triazole-5(4*H*)-thione dimethyl sulfoxide monosolvate

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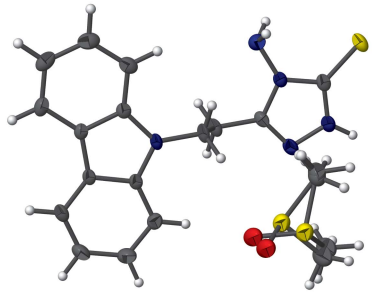
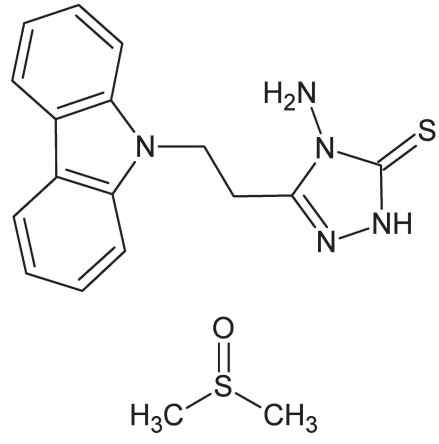
Structural data: full structural data are available from iucrdata.iucr.org

In the crystal of the title compound, $C_{16}H_{15}N_5S\cdot C_2H_6OS$, both the 1,2,4-triazole derivative molecules and the disordered [refined occupancy ratio = 0.604 (1):0.396 (1)] dimethyl sulfoxide solvent molecules form centrosymmetric dimers, by way of pairwise N—H···S and C—H···O hydrogen bonds, respectively. In the crystal, the two types of dimer are connected by N—H···O hydrogen bonds, forming infinite chains parallel to [101]. The packing is assisted by π–π stacking and C—H···π(ring) and N—H···π(ring) interactions.

3D view



Chemical scheme



Structure description

1,2,4-Triazole and its derivatives are found to be associated with various biological activities (Dundar *et al.*, 2007). For example, fluconazole is used as an antimicrobial drug, while vorozole, letrozole and anastrozole are non-steroidal and used for the treatment of cancer, and loreclezole is an anticonvulsant (Bekircan & Bektas, 2006). Moreover, 4-amino-1,2,4-triazoles are potentially good corrosion inhibitors (Dundar *et al.*, 2007). As part of our studies of triazole derivatives, we report herein the synthesis and crystal structure of the title 1,2,4-triazole derivative.

In the 1,2,4-triazole molecule (Fig. 1), the r.m.s. deviation from planarity of the carbazole moiety is 0.026 Å. The dihedral angle between its mean plane and the plane of the triazole ring is 2.01 (8)°. In the crystal, pairs of these molecules are linked into centrosymmetric dimers by pairs of N—H···S hydrogen bonds, giving rise to an $R_2^2(10)$ graph-set motif. The dimethyl sulfoxide solvent molecules are linked by pairs of C—

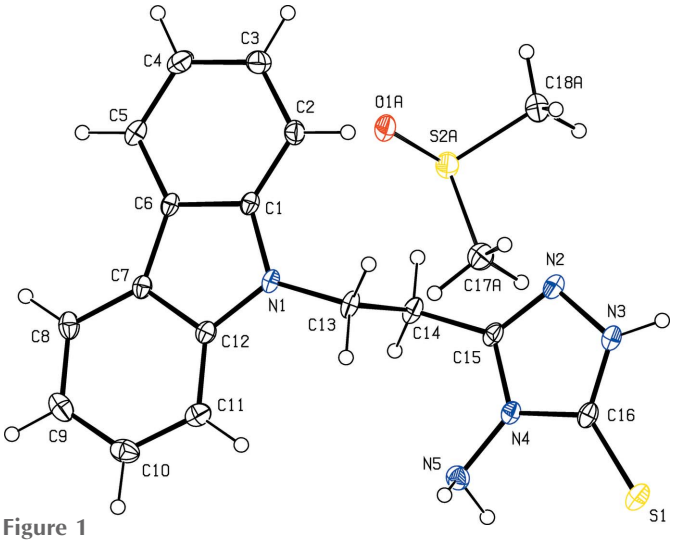


Figure 1
The title compound, with the atomic labelling and displacement ellipsoids drawn at the 30% probability level. The minor disorder component of the solvent molecule is not shown.

H···O hydrogen bonds into inversion dimers with a $R_2^2(8)$ motif (Table 1, Fig. 2). The two types of dimer are connected by N—H···O hydrogen bonds into chains running parallel to [101]. Between the chains, the primary intermolecular interactions are π–π-stacking between the N1/C1/C6/C7/C2 ring and the triazole ring at x, $-1 + y$, z [centroid-to-centroid

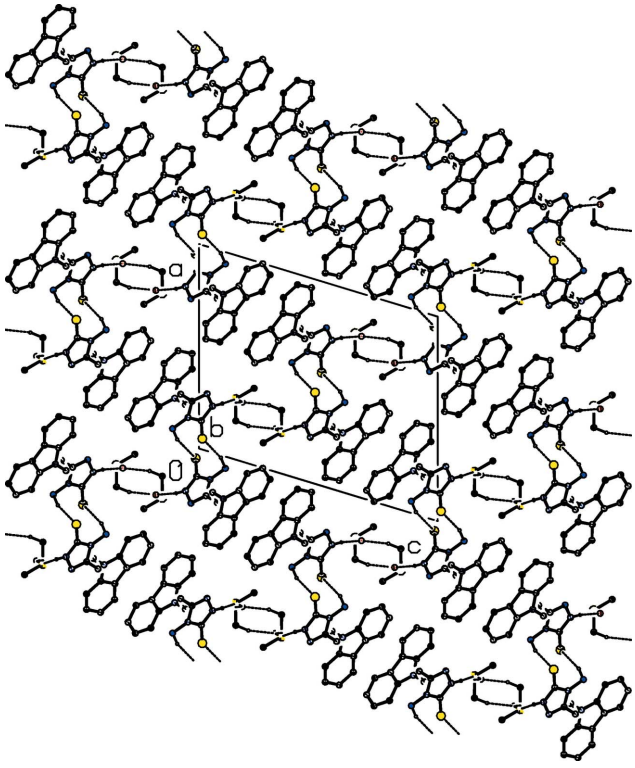


Figure 2
The packing of the title molecule, viewed along the b axis, showing the N—H···S and C—H···O interactions. Only the major component of the disordered DMSO solvent molecule is shown and H atoms have been omitted for clarity.

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

*Cg*4 is the centroid of the six-membered ring of the carbazole moiety.

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···O1A^{i}	0.91	1.92	2.818 (3)	171
N3—H3A···O1B^{i}	0.91	1.92	2.758 (4)	153
N5—H5B···S1^{ii}	0.91	2.51	3.3500 (17)	154
C17A—H17C···O1A^{iii}	0.98	2.43	3.242 (15)	140
C5—H5···$Cg4^{iv}$	0.95	2.54	3.452 (2)	161
N5—H5A···$Cg4^{i}$	0.91	2.60	3.2718 (18)	131

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{15}N_5S{\cdot}C_2H_6OS$
M_r	387.52
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	150
a, b, c (Å)	14.7620 (4), 7.3509 (2), 17.9987 (5)
β (°)	106.936 (1)
V (Å^3)	1868.41 (9)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	2.73
Crystal size (mm)	0.20 × 0.20 × 0.16
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.60, 0.67
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13596, 3572, 3350
R_{int}	0.027
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.618
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.046, 0.125, 1.04
No. of reflections	3572
No. of parameters	248
No. of restraints	6
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.57, −0.76

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012), *DIAMOND* (Brandenburg & Putz, 2012) and *PLATON* (Spek, 2009).

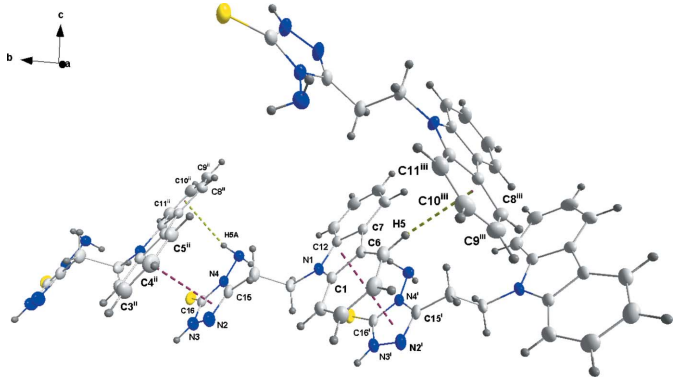


Figure 3
A view of the π–π stacking (purple dotted lines) and C—H···π(ring) (green dotted lines) interactions. [Symmetry codes: (i) $x, -1+y, z$; (ii) $x, 1+y, z$; (iii) $\frac{1}{2}-x, -\frac{1}{2}+y, \frac{3}{2}-z$.]

distance = 3.443 (1) Å; dihedral angle = 1.7 (1)°] and an offset π–π-stacking between the triazole ring and the C1–C6 ring at x, 1 + y, z [centroid-to-centroid distance = 3.706 (1) Å; dihedral angle = 1.0 (1)°, slippage 1.60 Å]. Additionally, there is a C5—H5$\cdots\pi$(ring) interaction and an N5—H5$A\cdots\pi$(ring) interaction (Table 1, Fig. 3).

Synthesis and crystallization

A mixture of 3-{2-[4a*H*-carbazol-9(9a*H*)-yl]ethyl}-1,2,4-oxadiazole-5-thiol (297 mg, 1 mmol) and an excess of hydrazine in ethanol (10 ml) was refluxed and monitored by TLC until completion. The solid product was collected by filtration and recrystallized from a dimethylsulfoxide solution to afford crystals of the title compound in a quality sufficient for X-ray diffraction measurements.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The solvent molecule was found to be disordered over two sets of sites with a refined ratio of 0.604 (1):0.396 (1). For refinement, restraints were applied so that the geometries of the two components were approximately the same. The (101) reflection was affected by the beam-stop and was omitted from the final cycles of refinement.

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x161855 [https://doi.org/10.1107/S2414314616018551]

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Crystal data

$C_{16}H_{15}N_5S\cdot C_2H_6OS$
M_r = 387.52
Monoclinic, $P2_1/n$
a = 14.7620 (4) Å
b = 7.3509 (2) Å
c = 17.9987 (5) Å
β = 106.936 (1)°
V = 1868.41 (9) Å^3
Z = 4
$F(000)$ = 816
D_x = 1.378 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9932 reflections
θ = 3.4–72.3°
μ = 2.73 mm^{-1}
T = 150 K
Block, colourless
0.20 × 0.20 × 0.16 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro-focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.60, T_{max} = 0.67
13596 measured reflections
3572 independent reflections
3350 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 72.2°, θ_{min} = 3.4°
h = −17→18
k = −9→9
l = −22→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.125
S = 1.04
3572 reflections
248 parameters
6 restraints
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0676P)^2 + 1.6793P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.76 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.44681 (3)	0.79061 (6)	0.48603 (3)	0.02910 (16)	
N1	0.29032 (11)	−0.0556 (2)	0.60195 (9)	0.0209 (3)	
N2	0.22063 (12)	0.4939 (2)	0.46625 (10)	0.0295 (4)	
N3	0.27261 (12)	0.6283 (2)	0.44330 (10)	0.0279 (4)	
H3A	0.2462	0.7031	0.4025	0.033*	
N4	0.36487 (11)	0.5161 (2)	0.54612 (9)	0.0216 (3)	
N5	0.44202 (12)	0.4762 (2)	0.61052 (10)	0.0269 (4)	
H5A	0.4621	0.5853	0.6333	0.032*	
H5B	0.4878	0.4298	0.5914	0.032*	
C1	0.20500 (13)	−0.1472 (2)	0.58859 (10)	0.0200 (4)	
C2	0.12152 (14)	−0.1248 (3)	0.52883 (11)	0.0259 (4)	
H2	0.1165	−0.0362	0.4894	0.031*	
C3	0.04597 (15)	−0.2363 (3)	0.52896 (13)	0.0315 (4)	
H3	−0.0117	−0.2245	0.4884	0.038*	
C4	0.05233 (14)	−0.3661 (3)	0.58726 (13)	0.0312 (5)	
H4	−0.0012	−0.4390	0.5862	0.037*	
C5	0.13586 (14)	−0.3891 (3)	0.64633 (12)	0.0259 (4)	
H5	0.1403	−0.4780	0.6856	0.031*	
C6	0.21365 (13)	−0.2795 (2)	0.64734 (10)	0.0197 (4)	
C7	0.30950 (13)	−0.2672 (2)	0.69755 (10)	0.0200 (4)	
C8	0.36090 (14)	−0.3633 (3)	0.76355 (11)	0.0262 (4)	
H8	0.3317	−0.4572	0.7846	0.031*	
C9	0.45494 (15)	−0.3189 (3)	0.79747 (12)	0.0322 (5)	
H9	0.4905	−0.3832	0.8423	0.039*	
C10	0.49835 (14)	−0.1808 (3)	0.76675 (12)	0.0320 (5)	
H10	0.5631	−0.1534	0.7911	0.038*	
C11	0.44939 (14)	−0.0828 (3)	0.70184 (12)	0.0275 (4)	
H11	0.4792	0.0112	0.6813	0.033*	
C12	0.35446 (13)	−0.1275 (2)	0.66761 (10)	0.0205 (4)	
C13	0.30589 (14)	0.0988 (2)	0.55708 (11)	0.0244 (4)	
H13A	0.2786	0.0719	0.5011	0.029*	
H13B	0.3748	0.1175	0.5672	0.029*	
C14	0.26134 (14)	0.2740 (2)	0.57672 (12)	0.0260 (4)	
H14A	0.1923	0.2565	0.5663	0.031*	
H14B	0.2886	0.3022	0.6326	0.031*	
C15	0.27912 (13)	0.4284 (2)	0.52932 (11)	0.0228 (4)	
C16	0.36048 (14)	0.6464 (2)	0.49055 (11)	0.0233 (4)	
S2A	0.20345 (6)	0.06746 (11)	0.34615 (5)	0.0318 (2)	0.6038 (10)
O1A	0.20930 (19)	−0.1242 (3)	0.31940 (15)	0.0372 (6)	0.6038 (10)
C17A	0.3100 (5)	0.1801 (13)	0.3459 (10)	0.0372 (5)	0.6038 (10)
H17A	0.3082	0.3061	0.3632	0.056*	0.6038 (10)
H17B	0.3641	0.1171	0.3812	0.056*	0.6038 (10)
H17C	0.3164	0.1792	0.2932	0.056*	0.6038 (10)
C18A	0.1235 (4)	0.1867 (10)	0.2692 (10)	0.0494 (18)	0.6038 (10)
H18A	0.1182	0.3129	0.2850	0.074*	0.6038 (10)

H18B	0.1468	0.1851	0.2235	0.074*	0.6038 (10)
H18C	0.0612	0.1284	0.2565	0.074*	0.6038 (10)
S2B	0.21829 (9)	0.05075 (17)	0.29873 (8)	0.0318 (2)	0.3962 (10)
O1B	0.1936 (3)	−0.0693 (5)	0.3583 (2)	0.0372 (6)	0.3962 (10)
C17B	0.3171 (8)	0.185 (2)	0.3500 (15)	0.0372 (5)	0.3962 (10)
H17D	0.3356	0.2655	0.3135	0.056*	0.3962 (10)
H17E	0.2998	0.2586	0.3892	0.056*	0.3962 (10)
H17F	0.3702	0.1053	0.3755	0.056*	0.3962 (10)
C18B	0.1314 (6)	0.2245 (18)	0.2758 (16)	0.0494 (18)	0.3962 (10)
H18D	0.1441	0.3067	0.2372	0.074*	0.3962 (10)
H18E	0.0686	0.1697	0.2547	0.074*	0.3962 (10)
H18F	0.1333	0.2931	0.3229	0.074*	0.3962 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0326 (3)	0.0194 (3)	0.0406 (3)	−0.00384 (17)	0.0189 (2)	−0.00093 (18)
N1	0.0257 (8)	0.0148 (7)	0.0238 (8)	−0.0011 (6)	0.0096 (6)	0.0035 (6)
N2	0.0305 (9)	0.0185 (8)	0.0378 (9)	−0.0036 (6)	0.0075 (7)	0.0033 (7)
N3	0.0322 (9)	0.0184 (8)	0.0316 (9)	−0.0024 (6)	0.0069 (7)	0.0046 (6)
N4	0.0246 (8)	0.0159 (7)	0.0255 (8)	0.0000 (6)	0.0090 (6)	0.0004 (6)
N5	0.0272 (8)	0.0247 (8)	0.0275 (8)	0.0031 (6)	0.0062 (7)	−0.0011 (6)
C1	0.0258 (9)	0.0145 (8)	0.0210 (8)	−0.0001 (7)	0.0088 (7)	−0.0007 (6)
C2	0.0307 (10)	0.0197 (9)	0.0255 (9)	0.0023 (7)	0.0054 (8)	0.0018 (7)
C3	0.0274 (10)	0.0267 (10)	0.0356 (11)	0.0001 (8)	0.0016 (8)	−0.0027 (8)
C4	0.0283 (10)	0.0254 (10)	0.0405 (11)	−0.0076 (8)	0.0111 (9)	−0.0034 (8)
C5	0.0311 (10)	0.0186 (9)	0.0310 (10)	−0.0034 (7)	0.0136 (8)	0.0004 (7)
C6	0.0262 (9)	0.0135 (8)	0.0211 (8)	0.0001 (6)	0.0097 (7)	−0.0005 (6)
C7	0.0264 (9)	0.0159 (8)	0.0193 (8)	0.0014 (7)	0.0093 (7)	−0.0012 (6)
C8	0.0364 (10)	0.0225 (9)	0.0208 (9)	0.0051 (8)	0.0103 (8)	0.0023 (7)
C9	0.0358 (11)	0.0339 (11)	0.0235 (9)	0.0115 (9)	0.0034 (8)	−0.0004 (8)
C10	0.0246 (9)	0.0359 (11)	0.0334 (11)	0.0032 (8)	0.0052 (8)	−0.0080 (9)
C11	0.0255 (9)	0.0255 (10)	0.0333 (10)	−0.0024 (8)	0.0113 (8)	−0.0048 (8)
C12	0.0241 (9)	0.0167 (8)	0.0221 (8)	0.0010 (7)	0.0088 (7)	−0.0023 (7)
C13	0.0352 (10)	0.0146 (8)	0.0281 (9)	−0.0004 (7)	0.0165 (8)	0.0033 (7)
C14	0.0311 (10)	0.0159 (9)	0.0351 (10)	−0.0005 (7)	0.0162 (8)	0.0016 (7)
C15	0.0253 (9)	0.0138 (8)	0.0317 (10)	−0.0003 (7)	0.0118 (8)	−0.0014 (7)
C16	0.0305 (9)	0.0152 (8)	0.0274 (9)	0.0011 (7)	0.0138 (8)	−0.0019 (7)
S2A	0.0371 (4)	0.0254 (4)	0.0298 (4)	−0.0003 (3)	0.0050 (3)	0.0024 (3)
O1A	0.0453 (12)	0.0199 (12)	0.0377 (14)	−0.0026 (9)	−0.0016 (11)	0.0041 (9)
C17A	0.0335 (14)	0.0370 (13)	0.0405 (17)	−0.0039 (10)	0.0097 (13)	0.0086 (12)
C18A	0.0376 (16)	0.037 (4)	0.064 (3)	−0.0008 (19)	−0.0012 (19)	0.020 (4)
S2B	0.0371 (4)	0.0254 (4)	0.0298 (4)	−0.0003 (3)	0.0050 (3)	0.0024 (3)
O1B	0.0453 (12)	0.0199 (12)	0.0377 (14)	−0.0026 (9)	−0.0016 (11)	0.0041 (9)
C17B	0.0335 (14)	0.0370 (13)	0.0405 (17)	−0.0039 (10)	0.0097 (13)	0.0086 (12)
C18B	0.0376 (16)	0.037 (4)	0.064 (3)	−0.0008 (19)	−0.0012 (19)	0.020 (4)

Geometric parameters (Å, º)

S1—C16	1.6776 (19)	C9—H9	0.9500
N1—C1	1.386 (2)	C10—C11	1.383 (3)
N1—C12	1.386 (2)	C10—H10	0.9500
N1—C13	1.450 (2)	C11—C12	1.396 (3)
N2—C15	1.302 (3)	C11—H11	0.9500
N2—N3	1.386 (2)	C13—C14	1.533 (3)
N3—C16	1.334 (3)	C13—H13A	0.9900
N3—H3A	0.9100	C13—H13B	0.9900
N4—C16	1.373 (2)	C14—C15	1.488 (3)
N4—C15	1.373 (2)	C14—H14A	0.9900
N4—N5	1.399 (2)	C14—H14B	0.9900
N5—H5A	0.9100	S2A—O1A	1.500 (2)
N5—H5B	0.9100	S2A—C18A	1.768 (7)
C1—C2	1.390 (3)	S2A—C17A	1.778 (7)
C1—C6	1.415 (2)	C17A—H17A	0.9800
C2—C3	1.385 (3)	C17A—H17B	0.9800
C2—H2	0.9500	C17A—H17C	0.9800
C3—C4	1.401 (3)	C18A—H18A	0.9800
C3—H3	0.9500	C18A—H18B	0.9800
C4—C5	1.384 (3)	C18A—H18C	0.9800
C4—H4	0.9500	S2B—O1B	1.512 (3)
C5—C6	1.399 (3)	S2B—C18B	1.772 (8)
C5—H5	0.9500	S2B—C17B	1.781 (8)
C6—C7	1.443 (3)	C17B—H17D	0.9800
C7—C8	1.400 (3)	C17B—H17E	0.9800
C7—C12	1.412 (2)	C17B—H17F	0.9800
C8—C9	1.383 (3)	C18B—H18D	0.9800
C8—H8	0.9500	C18B—H18E	0.9800
C9—C10	1.398 (3)	C18B—H18F	0.9800
C1—N1—C12	108.88 (14)	N1—C13—C14	112.40 (15)
C1—N1—C13	124.54 (15)	N1—C13—H13A	109.1
C12—N1—C13	126.43 (16)	C14—C13—H13A	109.1
C15—N2—N3	103.85 (16)	N1—C13—H13B	109.1
C16—N3—N2	113.64 (16)	C14—C13—H13B	109.1
C16—N3—H3A	124.3	H13A—C13—H13B	107.9
N2—N3—H3A	121.8	C15—C14—C13	110.45 (15)
C16—N4—C15	108.80 (16)	C15—C14—H14A	109.6
C16—N4—N5	127.16 (16)	C13—C14—H14A	109.6
C15—N4—N5	124.04 (15)	C15—C14—H14B	109.6
N4—N5—H5A	105.5	C13—C14—H14B	109.6
N4—N5—H5B	106.2	H14A—C14—H14B	108.1
H5A—N5—H5B	108.7	N2—C15—N4	110.67 (16)
N1—C1—C2	129.28 (17)	N2—C15—C14	126.79 (17)
N1—C1—C6	108.93 (15)	N4—C15—C14	122.47 (17)
C2—C1—C6	121.78 (17)	N3—C16—N4	103.03 (16)

C3—C2—C1	117.48 (18)	N3—C16—S1	130.04 (15)
C3—C2—H2	121.3	N4—C16—S1	126.93 (15)
C1—C2—H2	121.3	O1A—S2A—C18A	107.6 (5)
C2—C3—C4	121.76 (19)	O1A—S2A—C17A	107.6 (6)
C2—C3—H3	119.1	C18A—S2A—C17A	99.0 (4)
C4—C3—H3	119.1	S2A—C17A—H17A	109.5
C5—C4—C3	120.59 (18)	S2A—C17A—H17B	109.5
C5—C4—H4	119.7	H17A—C17A—H17B	109.5
C3—C4—H4	119.7	S2A—C17A—H17C	109.5
C4—C5—C6	118.93 (18)	H17A—C17A—H17C	109.5
C4—C5—H5	120.5	H17B—C17A—H17C	109.5
C6—C5—H5	120.5	S2A—C18A—H18A	109.5
C5—C6—C1	119.44 (17)	S2A—C18A—H18B	109.5
C5—C6—C7	134.08 (17)	H18A—C18A—H18B	109.5
C1—C6—C7	106.48 (15)	S2A—C18A—H18C	109.5
C8—C7—C12	119.46 (17)	H18A—C18A—H18C	109.5
C8—C7—C6	133.64 (17)	H18B—C18A—H18C	109.5
C12—C7—C6	106.89 (15)	O1B—S2B—C18B	106.1 (6)
C9—C8—C7	118.81 (19)	O1B—S2B—C17B	106.7 (7)
C9—C8—H8	120.6	C18B—S2B—C17B	98.6 (5)
C7—C8—H8	120.6	S2B—C17B—H17D	109.5
C8—C9—C10	120.90 (19)	S2B—C17B—H17E	109.5
C8—C9—H9	119.6	H17D—C17B—H17E	109.5
C10—C9—H9	119.6	S2B—C17B—H17F	109.5
C11—C10—C9	121.68 (19)	H17D—C17B—H17F	109.5
C11—C10—H10	119.2	H17E—C17B—H17F	109.5
C9—C10—H10	119.2	S2B—C18B—H18D	109.5
C10—C11—C12	117.43 (19)	S2B—C18B—H18E	109.5
C10—C11—H11	121.3	H18D—C18B—H18E	109.5
C12—C11—H11	121.3	S2B—C18B—H18F	109.5
N1—C12—C11	129.45 (17)	H18D—C18B—H18F	109.5
N1—C12—C7	108.81 (15)	H18E—C18B—H18F	109.5
C11—C12—C7	121.72 (17)		

C15—N2—N3—C16	−0.2 (2)	C13—N1—C12—C11	−6.5 (3)
C12—N1—C1—C2	−178.40 (18)	C1—N1—C12—C7	−0.4 (2)
C13—N1—C1—C2	5.8 (3)	C13—N1—C12—C7	175.25 (16)
C12—N1—C1—C6	0.7 (2)	C10—C11—C12—N1	−178.21 (18)
C13—N1—C1—C6	−175.03 (15)	C10—C11—C12—C7	−0.1 (3)
N1—C1—C2—C3	179.56 (18)	C8—C7—C12—N1	178.85 (16)
C6—C1—C2—C3	0.5 (3)	C6—C7—C12—N1	−0.05 (19)
C1—C2—C3—C4	0.6 (3)	C8—C7—C12—C11	0.4 (3)
C2—C3—C4—C5	−1.2 (3)	C6—C7—C12—C11	−178.51 (17)
C3—C4—C5—C6	0.6 (3)	C1—N1—C13—C14	75.0 (2)
C4—C5—C6—C1	0.5 (3)	C12—N1—C13—C14	−100.0 (2)
C4—C5—C6—C7	−178.90 (19)	N1—C13—C14—C15	−179.99 (15)
N1—C1—C6—C5	179.69 (16)	N3—N2—C15—N4	−0.2 (2)
C2—C1—C6—C5	−1.1 (3)	N3—N2—C15—C14	−177.15 (18)

N1—C1—C6—C7	−0.75 (19)	C16—N4—C15—N2	0.4 (2)
C2—C1—C6—C7	178.46 (17)	N5—N4—C15—N2	179.78 (16)
C5—C6—C7—C8	1.3 (4)	C16—N4—C15—C14	177.57 (16)
C1—C6—C7—C8	−178.19 (19)	N5—N4—C15—C14	−3.1 (3)
C5—C6—C7—C12	179.95 (19)	C13—C14—C15—N2	99.2 (2)
C1—C6—C7—C12	0.49 (19)	C13—C14—C15—N4	−77.4 (2)
C12—C7—C8—C9	−0.3 (3)	N2—N3—C16—N4	0.4 (2)
C6—C7—C8—C9	178.20 (19)	N2—N3—C16—S1	−179.43 (14)
C7—C8—C9—C10	0.0 (3)	C15—N4—C16—N3	−0.49 (19)
C8—C9—C10—C11	0.3 (3)	N5—N4—C16—N3	−179.81 (16)
C9—C10—C11—C12	−0.2 (3)	C15—N4—C16—S1	179.35 (14)
C1—N1—C12—C11	177.88 (18)	N5—N4—C16—S1	0.0 (3)

Hydrogen-bond geometry (Å, º)

Cg4 is the centroid of the six-membered ring of the carbazole moiety.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···O1*A*^{i}	0.91	1.92	2.818 (3)	171
N3—H3*A*···O1*B*^{i}	0.91	1.92	2.758 (4)	153
N5—H5*B*···S1^{ii}	0.91	2.51	3.3500 (17)	154
C17*A*—H17*C*···O1*A*^{iii}	0.98	2.43	3.242 (15)	140
C5—H5···*Cg*4^{iv}	0.95	2.54	3.452 (2)	161
N5—H5*A*···*Cg*4^{i}	0.91	2.60	3.2718 (18)	131

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