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5,5-Dimethyl-2-phenyl-4,5-dihydro-1,2,4-triazolo[1,5-*a*][1,3,5]triazin-7-amine[1]

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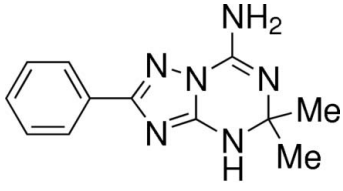
Key indicators: single-crystal X-ray study; T = 223 K; mean σ(C–C) = 0.002 Å; R factor = 0.046; wR factor = 0.121; data-to-parameter ratio = 16.5.

The title compound, $C_{12}H_{14}N_6$, was synthesized *via* cyclocondensation of 5-amino-1-guanyl-3-phenyl-1,2,4-triazole with acetone. Only one tautomeric form with an H atom at the triazine N atom was observed in the crystal structure. The compound crystallizes with two almost identical molecules in the asymmetric unit. In both molecules, the triazine ring adopts a conformation intermediate between a twist–boat and a half-boat. The crystal packing is stabilized by intermolecular N—H···N hydrogen bonds.

Related literature

The 1,2,4-triazolo[1,5-*a*][1,3,5]triazine (5-azapurine) heterocyclic system has been reviewed by Dolzhenko *et al.* (2006). The crystal structure of 7,7-dimethyl-2-phenyl-6,7-dihydro[1,2,4]triazolo[1,5-*a*][1,3,5]triazin-5-amine, which is regioisomeric with the title compound, (I), is reported in the previous paper (Dolzhenko, Tan *et al.*, 2007). For related literature, see also Dolzhenko, Dolzhenko & Chui (2007).



[1] Part 7 in the series 'Fused heterocyclic systems with *s*-triazine ring'. For Part 6, see Dolzhenko, Tan *et al.* (2007).

Experimental

Crystal data

$C_{12}H_{14}N_6$
M_r = 242.29
Triclinic, $P\overline{1}$
a = 9.7224 (5) Å
b = 11.9752 (6) Å
c = 12.4432 (6) Å
α = 112.200 (1)°
β = 103.737 (1)°
γ = 104.161 (1)°
V = 1209.58 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 223 (2) K
0.40 × 0.38 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.931, T_{max} = 0.980
15995 measured reflections
5549 independent reflections
4621 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.121
S = 1.06
5549 reflections
337 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5N···N7	0.874 (17)	2.150 (17)	2.9955 (16)	163 (2)
N6—H6A···N4^{i}	0.87	2.08	2.9491 (16)	172
N12—H12D···N10^{ii}	0.87	2.17	2.9844 (16)	156
N12—H12E···N2^{iii}	0.87	2.35	3.1119 (16)	146
N6—H6B···N8^{iv}	0.87	2.41	3.1751 (16)	147

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

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2003); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2380).

References

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supplementary materials

Acta Cryst. (2007). E**63**, o2797 [**doi:10.1107/S1600536807021022**]

5,5-Dimethyl-2-phenyl-4,5-dihydro-1,2,4-triazolo[1,5-*a*][1,3,5]triazin-7-amine

A. V. Dolzhenko, G. K. Tan, L. L. Koh, A. V. Dolzhenko and W. K. Chui

Comment

1,2,4-triazolo[1,5-*a*][1,3,5]triazines (5-azapurines) have been shown to exhibit many types of important biological activities (Dolzhenko *et al.*, 2006). As a part of our ongoing investigation on the derivatives of this heterocyclic system (Dolzhenko, Dolzhenko & Chui, 2007), we report herein the crystallographic study of the title compound (I) which is a regioisomer of previously described 7,7-dimethyl-2-phenyl-6,7-dihydro[1,2,4]triazolo[1,5-*a*][1,3,5]triazin- 5-amine (Dolzhenko, Tan *et al.*, 2007).

The title compound (I), $C_{12}H_{14}N_6$, was prepared by cyclocondensation of 5-amino-1-guanyl-3-phenyl-1,2,4-triazole with acetone. In general, the synthesized compound might be involved in annular tautomerism with three possible tautomeric forms (Fig. 1). However, only one tautomeric form *viz*. 5,5-dimethyl-2-phenyl-4,5-dihydro[1,2,4]triazolo[1,5-*a*][1,3,5]triazin- 7-amine (I) was observed in the crystal.

Compound (I) crystallizes with two independent molecules, *A* (Fig. 2) and *B* (Fig. 3), in the asymmetric unit (Fig. 4). The triazine rings of the molecules *A* and *B* adopt similar conformations best described as an intermediate between a twist-boat and a half-boat with atom C10 (C22) at the bow. The mean planes of the triazole and phenyl rings make a dihedral angles of 11.30 (5)° and 8.40 (6)° for the molecules *A* and *B*, respectively. The crystal packing is stabilized by intermolecular N—H···N hydrogen-bonds (Table 1)

Experimental

5-Amino-1-guanyl-3-phenyl-1,2,4-triazole (0.50 g, 2.5 mmol) was heated under reflux in acetone (8 ml) containing piperidine (0.05 ml, 0.5 mmol) for 12 h. After cooling, the precipitated solid was filtered, washed with acetone and recrystallized from ethanol (m.p. 482 K).

Refinement

Atom H5N and H11N were located in a difference map and refined isotropically. The remaining H atoms were placed in calculated positions (N—H = 0.87 Å and C—H = 0.94 or 0.97 Å), and included in the final cycles of refinement using a riding model, with U_{iso}(H) = 1.2U_{eq}(C, N) or 1.5U_{eq}(methyl C). A rotating group model was used for the methyl groups.

Figures

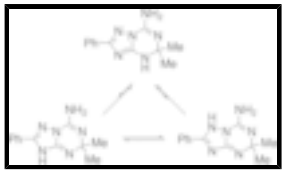


Fig. 1. The annular tautomerism in (I).
Fig. 2. One of the independent molecules of (I), molecule *A*, showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.
Fig. 3. One of the independent molecules of (I), molecule *B*, showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

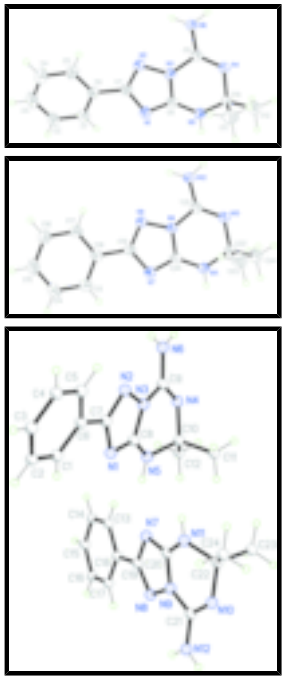


Fig. 4. The asymmetric unit of (I). Displacement ellipsoids are drawn at the 50% probability level.

5,5-Dimethyl-2-phenyl-4,5-dihydro-1,2,4-triazolo[1,5-*a*][1,3,5]triazin-\ 7-amine

Crystal data

$C_{12}H_{14}N_6$	$Z = 4$
$M_r = 242.29$	$F_{000} = 512$
Triclinic, $P\overline{1}$	$D_x = 1.331$ Mg m^{-3}
Hall symbol: -P 1	Melting point: 482 K
$a = 9.7224$ (5) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 11.9752$ (6) Å	Cell parameters from 4987 reflections
$c = 12.4432$ (6) Å	$\theta = 2.3$–27.4º
$\alpha = 112.200$ (1)º	$\mu = 0.09$ mm^{-1}
$\beta = 103.737$ (1)º	$T = 223$ (2) K
$\gamma = 104.161$ (1)º	Block, colourless
$V = 1209.58$ (10) Å^3	0.40 × 0.38 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer	4621 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.026$
$T = 223$(2) K	$\theta_{max} = 27.5$º
φ and ω scans	$\theta_{min} = 1.9$º
Absorption correction: multi-scan (SADABS; Sheldrick, 2001)	$h = -12 \rightarrow 12$
$T_{min} = 0.931$, $T_{max} = 0.980$	$k = -15 \rightarrow 15$

15995 measured reflections
5549 independent reflections

$l = -16 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.046$

$wR(F^2) = 0.121$

$S = 1.06$

5549 reflections

337 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0629P)^2 + 0.25P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.30$ e Å^{-3}

$\Delta\rho_{min} = -0.28$ e Å^{-3}

Extinction correction: none

Special details

Experimental. The su's on the cell Angles are rounded values.

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.43352 (12)	0.53590 (11)	0.34655 (11)	0.0283 (3)
N2	0.49145 (12)	0.35638 (10)	0.32551 (10)	0.0257 (2)
N3	0.62201 (12)	0.46598 (10)	0.37342 (10)	0.0254 (2)
N4	0.88222 (12)	0.58752 (11)	0.46028 (11)	0.0270 (2)
N5	0.69510 (13)	0.68668 (11)	0.43546 (12)	0.0316 (3)
H5N	0.6728 (19)	0.7549 (16)	0.4426 (15)	0.037 (4)*
N6	0.79574 (13)	0.37717 (11)	0.43315 (12)	0.0331 (3)
H6A	0.8877	0.3806	0.4644	0.040*
H6B	0.7177	0.3068	0.4073	0.040*
C1	0.11373 (16)	0.38462 (14)	0.25729 (13)	0.0317 (3)
H1	0.1475	0.4758	0.2972	0.038*
C2	−0.04123 (17)	0.31081 (16)	0.20182 (14)	0.0381 (3)

H2	−0.1120	0.3521	0.2045	0.046*
C3	−0.09205 (17)	0.17701 (16)	0.14279 (14)	0.0409 (4)
H3	−0.1972	0.1270	0.1044	0.049*
C4	0.01239 (18)	0.11703 (15)	0.14052 (15)	0.0406 (4)
H4	−0.0222	0.0258	0.1007	0.049*
C5	0.16773 (16)	0.18946 (14)	0.19612 (14)	0.0336 (3)
H5	0.2377	0.1474	0.1945	0.040*
C6	0.21989 (14)	0.32455 (13)	0.25427 (12)	0.0261 (3)
C7	0.38395 (14)	0.40484 (12)	0.31078 (12)	0.0248 (3)
C8	0.58319 (15)	0.57033 (12)	0.38609 (12)	0.0257 (3)
C9	0.77452 (14)	0.48004 (12)	0.42477 (12)	0.0244 (3)
C10	0.84763 (14)	0.68883 (13)	0.43383 (13)	0.0264 (3)
C11	0.85505 (18)	0.66838 (16)	0.30710 (14)	0.0391 (4)
H11A	0.9524	0.6628	0.3052	0.059*
H11B	0.8443	0.7409	0.2934	0.059*
H11C	0.7731	0.5884	0.2421	0.059*
C12	0.96425 (16)	0.82034 (14)	0.53578 (14)	0.0345 (3)
H12A	0.9585	0.8319	0.6159	0.052*
H12B	0.9430	0.8885	0.5191	0.052*
H12C	1.0657	0.8246	0.5374	0.052*
N7	0.64515 (12)	0.91698 (10)	0.41712 (10)	0.0253 (2)
N8	0.62672 (13)	1.09681 (10)	0.40021 (10)	0.0257 (2)
N9	0.58770 (13)	0.99346 (10)	0.28465 (10)	0.0257 (2)
N10	0.51588 (14)	0.88737 (11)	0.06878 (10)	0.0311 (3)
N11	0.55846 (14)	0.77685 (11)	0.19483 (11)	0.0289 (3)
H11N	0.562 (2)	0.7133 (19)	0.2025 (17)	0.050 (5)*
N12	0.50404 (15)	1.08991 (12)	0.16469 (11)	0.0351 (3)
H12D	0.4693	1.0909	0.0940	0.042*
H12E	0.5189	1.1555	0.2341	0.042*
C13	0.77339 (18)	1.06873 (15)	0.68743 (14)	0.0354 (3)
H13	0.7666	0.9821	0.6513	0.043*
C14	0.8361 (2)	1.14393 (17)	0.81604 (14)	0.0442 (4)
H14	0.8716	1.1077	0.8669	0.053*
C15	0.84680 (19)	1.27077 (16)	0.86998 (14)	0.0415 (4)
H15	0.8915	1.3216	0.9571	0.050*
C16	0.79161 (18)	1.32329 (15)	0.79563 (14)	0.0380 (3)
H16	0.7973	1.4096	0.8324	0.046*
C17	0.72806 (16)	1.24939 (13)	0.66731 (13)	0.0303 (3)
H17	0.6898	1.2854	0.6172	0.036*
C18	0.72058 (14)	1.12204 (12)	0.61204 (12)	0.0246 (3)
C19	0.66055 (14)	1.04497 (12)	0.47514 (12)	0.0229 (3)
C20	0.59803 (14)	0.88878 (12)	0.29832 (12)	0.0241 (3)
C21	0.53451 (15)	0.98768 (13)	0.16659 (12)	0.0259 (3)
C22	0.56405 (17)	0.78425 (13)	0.07957 (12)	0.0299 (3)
C23	0.7259 (2)	0.81007 (18)	0.08085 (16)	0.0448 (4)
H23A	0.7305	0.8189	0.0073	0.067*
H23B	0.7550	0.7382	0.0809	0.067*
H23C	0.7954	0.8896	0.1551	0.067*
C24	0.4530 (2)	0.65590 (15)	−0.03085 (14)	0.0453 (4)

H24A	0.3509	0.6423	−0.0298	0.068*
H24B	0.4821	0.5857	−0.0255	0.068*
H24C	0.4550	0.6576	−0.1078	0.068*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0236 (5)	0.0251 (6)	0.0355 (6)	0.0100 (5)	0.0086 (5)	0.0139 (5)
N2	0.0229 (5)	0.0228 (5)	0.0289 (6)	0.0065 (4)	0.0076 (4)	0.0118 (5)
N3	0.0225 (5)	0.0214 (5)	0.0321 (6)	0.0084 (4)	0.0077 (4)	0.0134 (5)
N4	0.0233 (5)	0.0258 (6)	0.0344 (6)	0.0108 (5)	0.0077 (5)	0.0171 (5)
N5	0.0244 (6)	0.0218 (6)	0.0500 (7)	0.0107 (5)	0.0111 (5)	0.0182 (5)
N6	0.0245 (6)	0.0271 (6)	0.0507 (7)	0.0111 (5)	0.0087 (5)	0.0231 (6)
C1	0.0294 (7)	0.0337 (7)	0.0312 (7)	0.0123 (6)	0.0099 (6)	0.0147 (6)
C2	0.0272 (7)	0.0524 (9)	0.0390 (8)	0.0170 (7)	0.0117 (6)	0.0242 (7)
C3	0.0247 (7)	0.0509 (10)	0.0348 (8)	0.0019 (6)	0.0068 (6)	0.0178 (7)
C4	0.0362 (8)	0.0330 (8)	0.0391 (8)	0.0014 (6)	0.0133 (7)	0.0110 (7)
C5	0.0314 (7)	0.0307 (7)	0.0369 (8)	0.0098 (6)	0.0142 (6)	0.0141 (6)
C6	0.0247 (6)	0.0289 (7)	0.0249 (6)	0.0088 (5)	0.0094 (5)	0.0131 (5)
C7	0.0250 (6)	0.0255 (6)	0.0243 (6)	0.0095 (5)	0.0089 (5)	0.0119 (5)
C8	0.0261 (6)	0.0247 (6)	0.0287 (7)	0.0123 (5)	0.0091 (5)	0.0138 (5)
C9	0.0234 (6)	0.0265 (6)	0.0258 (6)	0.0118 (5)	0.0083 (5)	0.0135 (5)
C10	0.0226 (6)	0.0254 (6)	0.0337 (7)	0.0102 (5)	0.0079 (5)	0.0170 (6)
C11	0.0401 (8)	0.0437 (9)	0.0374 (8)	0.0147 (7)	0.0127 (7)	0.0240 (7)
C12	0.0282 (7)	0.0275 (7)	0.0421 (8)	0.0079 (6)	0.0079 (6)	0.0150 (6)
N7	0.0292 (6)	0.0240 (5)	0.0253 (5)	0.0106 (4)	0.0097 (5)	0.0136 (5)
N8	0.0303 (6)	0.0235 (5)	0.0230 (5)	0.0106 (5)	0.0087 (4)	0.0108 (4)
N9	0.0338 (6)	0.0217 (5)	0.0234 (5)	0.0120 (5)	0.0089 (5)	0.0120 (4)
N10	0.0444 (7)	0.0268 (6)	0.0256 (6)	0.0168 (5)	0.0106 (5)	0.0145 (5)
N11	0.0423 (7)	0.0218 (6)	0.0277 (6)	0.0149 (5)	0.0131 (5)	0.0145 (5)
N12	0.0555 (8)	0.0305 (6)	0.0254 (6)	0.0247 (6)	0.0116 (5)	0.0154 (5)
C13	0.0460 (9)	0.0344 (8)	0.0307 (7)	0.0201 (7)	0.0126 (6)	0.0175 (6)
C14	0.0575 (10)	0.0513 (10)	0.0294 (8)	0.0273 (8)	0.0115 (7)	0.0226 (7)
C15	0.0479 (9)	0.0456 (9)	0.0238 (7)	0.0158 (7)	0.0103 (6)	0.0115 (7)
C16	0.0460 (9)	0.0313 (8)	0.0320 (8)	0.0129 (7)	0.0155 (7)	0.0104 (6)
C17	0.0342 (7)	0.0301 (7)	0.0305 (7)	0.0134 (6)	0.0132 (6)	0.0161 (6)
C18	0.0227 (6)	0.0271 (7)	0.0258 (6)	0.0090 (5)	0.0099 (5)	0.0136 (5)
C19	0.0204 (6)	0.0227 (6)	0.0277 (6)	0.0074 (5)	0.0092 (5)	0.0141 (5)
C20	0.0244 (6)	0.0233 (6)	0.0286 (6)	0.0097 (5)	0.0099 (5)	0.0153 (5)
C21	0.0286 (7)	0.0258 (6)	0.0250 (6)	0.0105 (5)	0.0080 (5)	0.0144 (5)
C22	0.0424 (8)	0.0254 (7)	0.0255 (7)	0.0158 (6)	0.0121 (6)	0.0135 (6)
C23	0.0535 (10)	0.0545 (10)	0.0475 (9)	0.0301 (9)	0.0285 (8)	0.0322 (8)
C24	0.0689 (12)	0.0285 (8)	0.0302 (8)	0.0170 (8)	0.0100 (8)	0.0111 (6)

Geometric parameters (Å, °)

N1—C8	1.3200 (17)	N7—C20	1.3170 (17)
N1—C7	1.3761 (17)	N7—C19	1.3758 (16)
N2—C7	1.3224 (17)	N8—C19	1.3246 (16)

N2—N3	1.3869 (15)	N8—N9	1.3818 (15)
N3—C8	1.3561 (16)	N9—C20	1.3508 (16)
N3—C9	1.4078 (16)	N9—C21	1.4054 (16)
N4—C9	1.2803 (17)	N10—C21	1.2811 (17)
N4—C10	1.4636 (16)	N10—C22	1.4631 (17)
N5—C8	1.3403 (17)	N11—C20	1.3457 (17)
N5—C10	1.4819 (17)	N11—C22	1.4828 (17)
N5—H5N	0.874 (17)	N11—H11N	0.810 (19)
N6—C9	1.3350 (16)	N12—C21	1.3353 (17)
N6—H6A	0.87	N12—H12D	0.87
N6—H6B	0.87	N12—H12E	0.87
C1—C2	1.386 (2)	C13—C14	1.387 (2)
C1—C6	1.3948 (19)	C13—C18	1.3912 (19)
C1—H1	0.94	C13—H13	0.94
C2—C3	1.379 (2)	C14—C15	1.374 (2)
C2—H2	0.94	C14—H14	0.94
C3—C4	1.379 (2)	C15—C16	1.381 (2)
C3—H3	0.94	C15—H15	0.94
C4—C5	1.386 (2)	C16—C17	1.382 (2)
C4—H4	0.94	C16—H16	0.94
C5—C6	1.3919 (19)	C17—C18	1.3905 (19)
C5—H5	0.94	C17—H17	0.94
C6—C7	1.4728 (18)	C18—C19	1.4732 (18)
C10—C12	1.5193 (19)	C22—C24	1.518 (2)
C10—C11	1.524 (2)	C22—C23	1.523 (2)
C11—H11A	0.97	C23—H23A	0.97
C11—H11B	0.97	C23—H23B	0.97
C11—H11C	0.97	C23—H23C	0.97
C12—H12A	0.97	C24—H24A	0.97
C12—H12B	0.97	C24—H24B	0.97
C12—H12C	0.97	C24—H24C	0.97
C8—N1—C7	102.36 (11)	C20—N7—C19	102.43 (10)
C7—N2—N3	101.17 (10)	C19—N8—N9	101.35 (10)
C8—N3—N2	109.71 (10)	C20—N9—N8	109.76 (10)
C8—N3—C9	121.45 (11)	C20—N9—C21	122.04 (11)
N2—N3—C9	127.86 (10)	N8—N9—C21	128.07 (10)
C9—N4—C10	119.88 (11)	C21—N10—C22	120.53 (11)
C8—N5—C10	117.54 (11)	C20—N11—C22	117.96 (11)
C8—N5—H5N	120.0 (11)	C20—N11—H11N	118.6 (13)
C10—N5—H5N	118.8 (11)	C22—N11—H11N	119.8 (13)
C9—N6—H6A	120.0	C21—N12—H12D	120.0
C9—N6—H6B	120.0	C21—N12—H12E	120.0
H6A—N6—H6B	120.0	H12D—N12—H12E	120.0
C2—C1—C6	120.45 (14)	C14—C13—C18	119.75 (14)
C2—C1—H1	119.8	C14—C13—H13	120.1
C6—C1—H1	119.8	C18—C13—H13	120.1
C3—C2—C1	120.26 (14)	C15—C14—C13	120.70 (14)
C3—C2—H2	119.9	C15—C14—H14	119.7
C1—C2—H2	119.9	C13—C14—H14	119.7

C2—C3—C4	119.56 (14)	C14—C15—C16	119.75 (14)
C2—C3—H3	120.2	C14—C15—H15	120.1
C4—C3—H3	120.2	C16—C15—H15	120.1
C3—C4—C5	120.88 (15)	C15—C16—C17	120.25 (14)
C3—C4—H4	119.6	C15—C16—H16	119.9
C5—C4—H4	119.6	C17—C16—H16	119.9
C4—C5—C6	119.89 (14)	C16—C17—C18	120.23 (13)
C4—C5—H5	120.1	C16—C17—H17	119.9
C6—C5—H5	120.1	C18—C17—H17	119.9
C5—C6—C1	118.95 (13)	C17—C18—C13	119.28 (13)
C5—C6—C7	121.50 (12)	C17—C18—C19	120.54 (12)
C1—C6—C7	119.54 (12)	C13—C18—C19	120.16 (12)
N2—C7—N1	116.11 (11)	N8—C19—N7	115.68 (11)
N2—C7—C6	123.05 (12)	N8—C19—C18	121.99 (11)
N1—C7—C6	120.78 (11)	N7—C19—C18	122.21 (11)
N1—C8—N5	130.97 (12)	N7—C20—N11	130.98 (12)
N1—C8—N3	110.62 (11)	N7—C20—N9	110.77 (11)
N5—C8—N3	118.40 (12)	N11—C20—N9	118.24 (11)
N4—C9—N6	124.39 (12)	N10—C21—N12	123.95 (12)
N4—C9—N3	119.53 (11)	N10—C21—N9	119.94 (12)
N6—C9—N3	116.08 (11)	N12—C21—N9	116.11 (11)
N4—C10—N5	110.85 (10)	N10—C22—N11	111.25 (11)
N4—C10—C12	108.60 (11)	N10—C22—C24	107.89 (12)
N5—C10—C12	107.48 (11)	N11—C22—C24	107.66 (12)
N4—C10—C11	109.05 (11)	N10—C22—C23	109.33 (12)
N5—C10—C11	110.48 (11)	N11—C22—C23	109.52 (12)
C12—C10—C11	110.36 (12)	C24—C22—C23	111.19 (13)
C10—C11—H11A	109.5	C22—C23—H23A	109.5
C10—C11—H11B	109.5	C22—C23—H23B	109.5
H11A—C11—H11B	109.5	H23A—C23—H23B	109.5
C10—C11—H11C	109.5	C22—C23—H23C	109.5
H11A—C11—H11C	109.5	H23A—C23—H23C	109.5
H11B—C11—H11C	109.5	H23B—C23—H23C	109.5
C10—C12—H12A	109.5	C22—C24—H24A	109.5
C10—C12—H12B	109.5	C22—C24—H24B	109.5
H12A—C12—H12B	109.5	H24A—C24—H24B	109.5
C10—C12—H12C	109.5	C22—C24—H24C	109.5
H12A—C12—H12C	109.5	H24A—C24—H24C	109.5
H12B—C12—H12C	109.5	H24B—C24—H24C	109.5
C7—N2—N3—C8	1.37 (13)	C19—N8—N9—C20	1.11 (13)
C7—N2—N3—C9	170.10 (12)	C19—N8—N9—C21	177.04 (12)
C6—C1—C2—C3	−0.1 (2)	C18—C13—C14—C15	−0.1 (3)
C1—C2—C3—C4	0.7 (2)	C13—C14—C15—C16	1.4 (3)
C2—C3—C4—C5	−0.4 (2)	C14—C15—C16—C17	−1.1 (2)
C3—C4—C5—C6	−0.5 (2)	C15—C16—C17—C18	−0.6 (2)
C4—C5—C6—C1	1.1 (2)	C16—C17—C18—C13	2.0 (2)
C4—C5—C6—C7	−177.98 (13)	C16—C17—C18—C19	−176.71 (13)
C2—C1—C6—C5	−0.8 (2)	C14—C13—C18—C17	−1.6 (2)
C2—C1—C6—C7	178.33 (13)	C14—C13—C18—C19	177.07 (14)

N3—N2—C7—N1	−0.93 (14)	N9—N8—C19—N7	−0.54 (14)
N3—N2—C7—C6	176.30 (11)	N9—N8—C19—C18	175.52 (11)
C8—N1—C7—N2	0.12 (15)	C20—N7—C19—N8	−0.24 (14)
C8—N1—C7—C6	−177.18 (12)	C20—N7—C19—C18	−176.29 (11)
C5—C6—C7—N2	−9.5 (2)	C17—C18—C19—N8	7.11 (19)
C1—C6—C7—N2	171.34 (12)	C13—C18—C19—N8	−171.56 (13)
C5—C6—C7—N1	167.56 (13)	C17—C18—C19—N7	−177.08 (12)
C1—C6—C7—N1	−11.56 (19)	C13—C18—C19—N7	4.24 (19)
C7—N1—C8—N5	−178.18 (14)	C19—N7—C20—N11	−177.73 (14)
C7—N1—C8—N3	0.80 (14)	C19—N7—C20—N9	0.96 (14)
C10—N5—C8—N1	−161.07 (14)	C22—N11—C20—N7	−158.17 (13)
C10—N5—C8—N3	20.01 (18)	C22—N11—C20—N9	23.22 (18)
N2—N3—C8—N1	−1.44 (15)	N8—N9—C20—N7	−1.38 (15)
C9—N3—C8—N1	−171.02 (11)	C21—N9—C20—N7	−177.60 (11)
N2—N3—C8—N5	177.69 (11)	N8—N9—C20—N11	177.50 (11)
C9—N3—C8—N5	8.11 (19)	C21—N9—C20—N11	1.28 (19)
C10—N4—C9—N6	172.98 (13)	C22—N10—C21—N12	174.81 (13)
C10—N4—C9—N3	−7.26 (19)	C22—N10—C21—N9	−6.3 (2)
C8—N3—C9—N4	−15.29 (19)	C20—N9—C21—N10	−10.5 (2)
N2—N3—C9—N4	177.17 (12)	N8—N9—C21—N10	174.01 (13)
C8—N3—C9—N6	164.48 (12)	C20—N9—C21—N12	168.51 (12)
N2—N3—C9—N6	−3.06 (19)	N8—N9—C21—N12	−7.0 (2)
C9—N4—C10—N5	32.61 (17)	C21—N10—C22—N11	28.29 (18)
C9—N4—C10—C12	150.47 (13)	C21—N10—C22—C24	146.15 (14)
C9—N4—C10—C11	−89.23 (15)	C21—N10—C22—C23	−92.80 (16)
C8—N5—C10—N4	−39.04 (16)	C20—N11—C22—N10	−36.86 (17)
C8—N5—C10—C12	−157.58 (12)	C20—N11—C22—C24	−154.87 (13)
C8—N5—C10—C11	81.96 (15)	C20—N11—C22—C23	84.11 (15)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5N···N7	0.874 (17)	2.150 (17)	2.9955 (16)	163 (2)
N6—H6A···N4^{i}	0.87	2.08	2.9491 (16)	172
N12—H12D···N10^{ii}	0.87	2.17	2.9844 (16)	156
N12—H12E···N2^{iii}	0.87	2.35	3.1119 (16)	146
N6—H6B···N8^{iv}	0.87	2.41	3.1751 (16)	147

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

Fig. 1

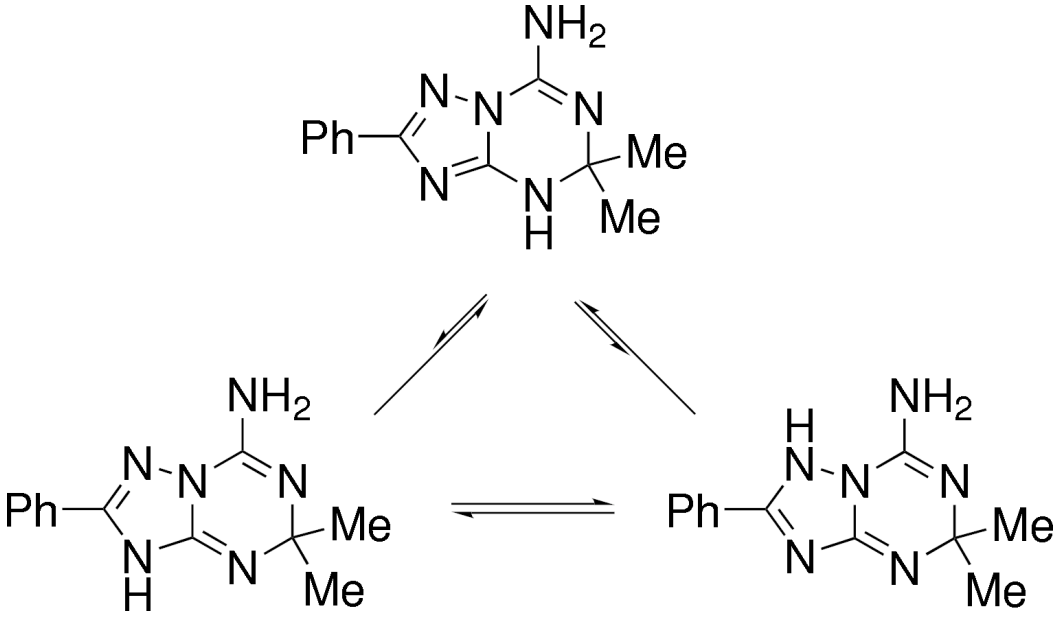


Fig. 2

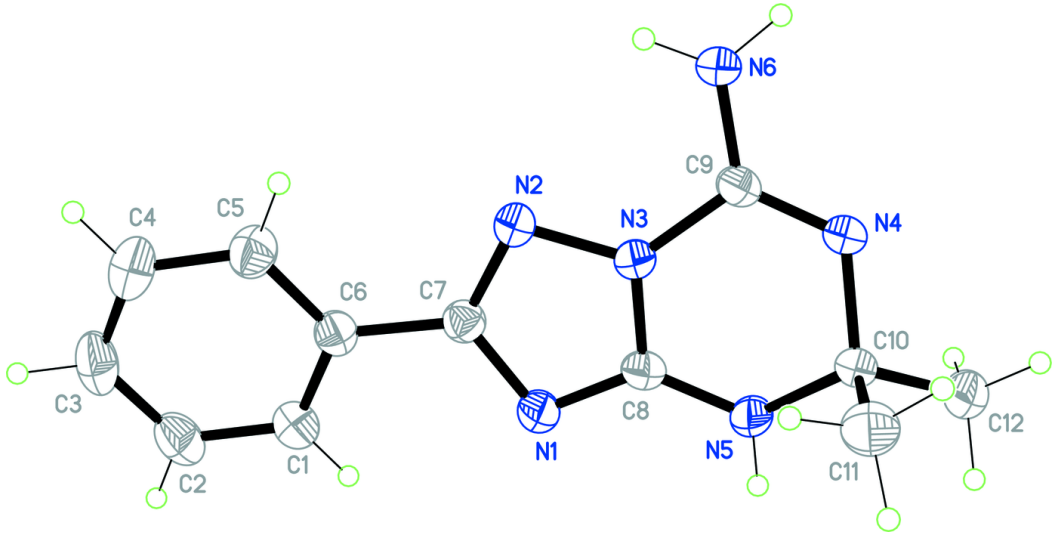
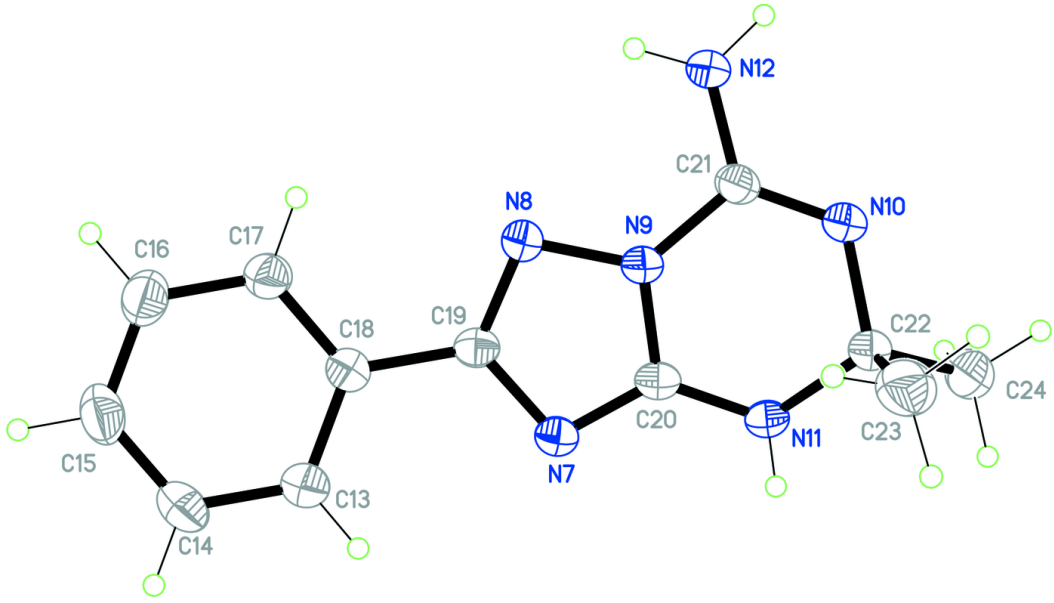


Fig. 3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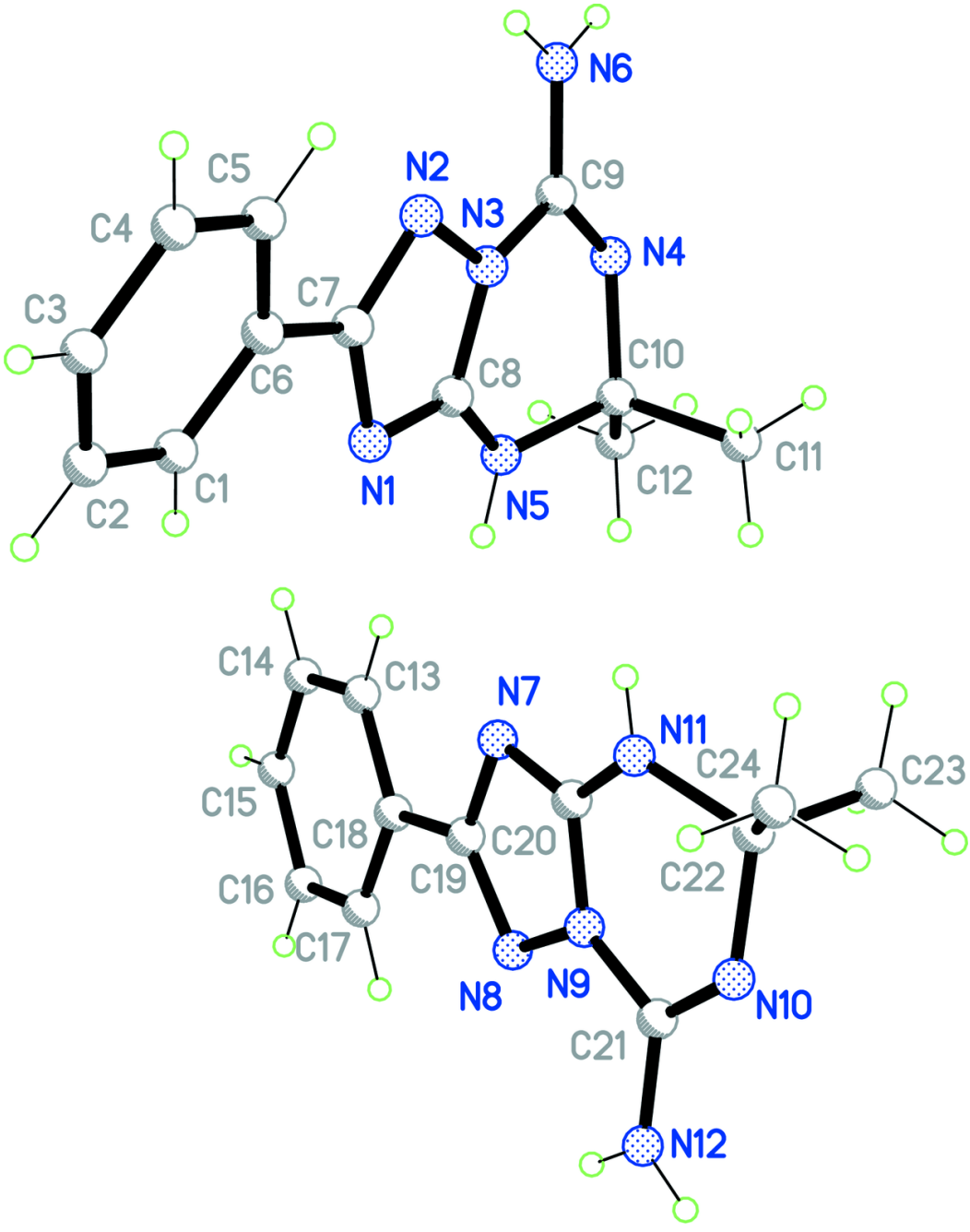
C21
N8
N9
N10
C16
C17
C18
C19
C22
C24
C15
C20
C23
N11
N7
C13
C14

Fig. 4


N6
C5
N2
C9
C4
N3
N4
C7
C3
C10
C6
C8
C11
C1
N1
N5
C12
C2
C14
C13
N7
N11
C24
C23
C15
C18
C20
C19
C22
C16
C17
N8
N9
N10
C21
N12