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N-[3-Methyl-1-phenyl-1-(1*H*-tetrazol-1-yl)butan-2-yl]acetamide

data reports

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In the molecule of the title compound, $C_{14}H_{19}N_5O$, the dihedral angle formed between the tetrazole and phenyl rings is 68.39 (4)°. In the crystal, molecules are linked by N-H···N, C-H···N and C-H···O hydrogen bonds to form twodimensional networks extending parallel to the *bc* plane.



Structure description

Compounds containing a tetrazole ring have attracted much attention in medicinal chemistry (Alam & Nasrollahzadeh, 2009). Tetrazoles are reported to exhibits antihypertensive (Sharma *et al.*, 2010), antimicrobial (Yildirir *et al.*, 2009), antibacterial, antifungal (Dhayanithi *et al.*, 2011) and anticancer activities (Bhaskar & Mohite, 2010). These functional units exhibit strong networking ability as ligands. They act as mono-, bior multidentate ligands due to the electron-donating nature of the four nitrogen atoms in the tetrazole moiety (Wang *et al.*, 2005).

In the title compound (Fig. 1), the bond between the two chiral carbons C7 and C8 acts as the bridge connecting the phenyl ring, the 1-*H* tetrazole ring and the acetamide unit. The dihedral angle between the tetrazole ring (N1–N4, C14) and the phenyl ring (C1–C6) is $68.39 (4)^{\circ}$. The mean plane through the acetamide unit (N5, C12, C13, O1) forms dihedral angles of 62.00 (6) and $13.23 (6)^{\circ}$ with the tetrazole and phenyl rings, respectively.

In the crystal, the molecules are linked through $C-H\cdots O$, $C-H\cdots N$ and $N-H\cdots N$ hydrogen bonds (Table 1) into two-dimensional networks extending parallel to the *bc* plane (Fig. 2).







The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level. H atoms are shown as small spheres of arbitrary radius.

Synthesis and crystallization

A Mannich condensation reaction involving benzaldehye (200 mmol), isobutyl methyl ketone (100 mmol) and ammonium acetate (100 mmol) in 70 ml methanol at 70°C for 2 h afforded the respective piperidinone as crystals. The crystals were washed with methanol, dried completely under vacuum, then converted into the hydrochloride form by dissolving them in 30 ml ethanol and 20 ml ether and adding an equivalent volume of concentrated hydrochloric acid dropwise. 2 g of the precipitate obtained was gradually added to a beaker containing 10 ml of concentrated sulfuric acid in icecold condition, dissolved thoroughly and kept at room temperature with continuous stirring. 0.65 g of sodium azide was then added in small quantities to the beaker. On addition



Figure 2

Partial crystal packing of the title compound showing the formation of a two-dimensional network parallel to the *bc* plane *via* $N-H\cdots N$, $C-H\cdots O$ and $C-H\cdots N$ hydrogen bonds (dashed lines).

| Table 1 | | |
|--------------|----------------|--------|
| Hydrogen-bor | nd geometry (A | Å, °). |

| $D - H \cdots A$ | D-H | $H \cdot \cdot \cdot A$ | $D \cdots A$ | $D - H \cdot \cdot \cdot A$ |
|---|------------------------------------|------------------------------------|--|---------------------------------|
| $N5-H5A\cdots N2^{i}$ $C6-H6\cdots O1^{ii}$ $C7-H7\cdots N3^{i}$ $C14-H14\cdots O1^{ii}$ | 0.844 (18) 0.93 0.98 0.93 | 2.452 (18) 2.43 2.48 2.27 | 3.2579 (17) 3.356 (2) 3.4055 (19) 3.1728 (19) | 160.0 (15) 171 157 163 |

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

 Table 2

 Experimental details.

| Crystal data | |
|--|--|
| Chemical formula | $C_{14}H_{19}N_5O$ |
| Mr | 273.34 |
| Crystal system, space group | Monoclinic, $P2_1/c$ |
| Temperature (K) | 296 |
| a, b, c (Å) | 9.7056 (6), 7.7663 (5), 20.2620 (9) |
| β (°) | 93.490 (2) |
| $V(Å^3)$ | 1524.45 (15) |
| Ζ | 4 |
| Radiation type | Μο Κα |
| $\mu \text{ (mm}^{-1})$ | 0.08 |
| Crystal size (mm) | $0.35 \times 0.30 \times 0.30$ |
| Data collection | |
| Diffractometer | Bruker Kappa APEXII CCD |
| Absorption correction | Multi-scan (<i>SADABS</i> ; Bruker, 2004) |
| T_{\min}, T_{\max} | 0.740, 0.976 |
| No. of measured, independent and observed $[I > 2\sigma(I)]$ reflections | 10998, 3760, 2712 |
| R _{int} | 0.020 |
| $(\sin \theta / \lambda)_{\max} (\text{\AA}^{-1})$ | 0.667 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)], wR(F^2), S$ | 0.047, 0.134, 1.02 |
| No. of reflections | 3760 |
| No. of parameters | 188 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta \rho_{\rm max}, \Delta \rho_{\rm min} \ ({ m e} \ { m \AA}^{-3})$ | 0.23, -0.17 |
| | |

Computer programs: *APEX2* and *SAINT* (Bruker, 2004), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

of sodium azide, a foam formed which subsequently subsided due to liberation of nitrogen. The solution was transferred into a beaker containing ice and neutralized with 4 M sodium hydroxide. The white precipitate formed was filtered through a Buchner funnel, vacuum dried and recrystallized with ethanol. The resulting lactam was cleaved under acidic conditions (6 M HCl) to form the substituted vicinal diamine. Conversion of the hydrochloride salt of the vicinal diamine into the free diamine was performed using 2 mol of sodium acetate. The vicinal diamine was then converted into acetylated 1-substituted tetrazole in the presence of 2 mol of sodium azide and 2 mol of triethyl orthoformate at 60°C in a glacial acetic acid medium. The compound obtained was then dissolved in methanol, transferred to a 15 ml vial, and the vial wrapped with tissue paper for controlled evaporation of the solvent without contamination. Single crystals suitable for X-ray analysis were formed after three days.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x161810 [https://doi.org/10.1107/S2414314616018101]

N-[3-Methyl-1-phenyl-1-(1H-tetrazol-1-yl)butan-2-yl]acetamide

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N-[3-Methyl-1-phenyl-1-(1H-tetrazol-1-yl)butan-2-yl]acetamide

Crystal data

C₁₄H₁₉N₅O $M_r = 273.34$ Monoclinic, $P2_1/c$ Hall symbol: -P 2ybc a = 9.7056 (6) Å b = 7.7663 (5) Å c = 20.2620 (9) Å $\beta = 93.490$ (2)° V = 1524.45 (15) Å³ Z = 4

Data collection

Bruker Kappa APEXII CCD diffractometer Radiation source: fine-focus sealed tube Graphite monochromator Bruker axs kappa apex2 CCD Diffractometer scans Absorption correction: multi-scan (SADABS; Bruker, 2004) $T_{min} = 0.740, T_{max} = 0.976$

Refinement

Refinement on F^2 Least-squares matrix: full $R[F^2 > 2\sigma(F^2)] = 0.047$ $wR(F^2) = 0.134$ S = 1.023760 reflections 188 parameters 0 restraints Primary atom site location: structure-invariant direct methods F(000) = 584 $D_x = 1.191 \text{ Mg m}^{-3}$ Melting point: 393 K Mo Ka radiation, $\lambda = 0.71073 \text{ Å}$ Cell parameters from 3760 reflections $\theta = 2.8-28.3^{\circ}$ $\mu = 0.08 \text{ mm}^{-1}$ T = 296 KBlock, colourless $0.35 \times 0.30 \times 0.30 \text{ mm}$

10998 measured reflections 3760 independent reflections 2712 reflections with $I > 2\sigma(I)$ $R_{int} = 0.020$ $\theta_{max} = 28.3^{\circ}, \ \theta_{min} = 2.8^{\circ}$ $h = -12 \rightarrow 12$ $k = -10 \rightarrow 10$ $l = -26 \rightarrow 16$

Secondary atom site location: difference Fourier map Hydrogen site location: mixed H atoms treated by a mixture of independent and constrained refinement $w = 1/[\sigma^2(F_o^2) + (0.0588P)^2 + 0.4088P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{max} = 0.010$ $\Delta\rho_{max} = 0.23$ e Å⁻³ $\Delta\rho_{min} = -0.17$ 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.

| O1 0.61825 (12) 0.64603 (18) 0.04105 (5) 0.0500 (3) N1 0.43416 (11) 0.3137 (2) 0.21287 (6) 0.0555 (4) N3 0.57528 (16) 0.2002 (2) 0.19824 (7) 0.0605 (4) N4 0.58598 (13) 0.19027 (18) 0.13256 (7) 0.0484 (3) N5 0.50558 (12) 0.72547 (16) 0.12972 (6) 0.0338 (3) C1 0.18648 (14) 0.4056 (18) 0.13633 (7) 0.0374 (3) C2 0.09223 (18) 0.4295 (3) 0.18515 (9) 0.0616 (5) L2 0.0152 0.4707 0.2275 0.074* C3 -0.0371 (2) 0.3568 (3) 0.17039 (13) 0.0847 (7) H3 -0.1001 0.3499 0.2031 0.102* C4 -0.07241 (19) 0.2958 (3) 0.10887 (13) 0.0788 (6) H4 -0.150 0.2474 0.0995 0.095* C5 0.2009 (18) 0.3616 (3) 0.04608 (10) 0.031 (5) H5 -0.038 0.2645 0 | | x | у | Ζ | $U_{ m iso}$ */ $U_{ m eq}$ | |
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| C10.18648 (14)0.44056 (18)0.13683 (7)0.0374 (3)C20.09223 (18)0.4295 (3)0.18515 (9)0.0616 (5)H20.11520.47070.22750.074*C3-0.0371 (2)0.3568 (3)0.17039 (13)0.0847 (7)H3-0.10010.34990.20310.102*C4-0.07241 (19)0.2958 (3)0.10887 (13)0.0788 (6)H4-0.15900.24740.09950.095*C50.02009 (18)0.3061 (3)0.06068 (10)0.0631 (5)H5-0.00380.26450.01850.076*C60.14894 (15)0.3779 (2)0.07445 (8)0.0462 (4)H60.21110.38420.04140.055*C70.32751 (14)0.51735 (18)0.15342 (6)0.0349 (3)H70.32680.56740.19780.042*C80.37089 (14)0.65989 (18)0.10615 (6)0.0349 (3)H80.38170.60630.06300.042*C90.26314 (16)0.8039 (2)0.0599 (7)0.448 (4)H90.17490.74950.08220.054*C100.2413 (2)0.9010 (3)0.15828 (9)0.0667 (5)H10A0.32420.9215 (2)0.40006 (8)0.0666 (5)H10B0.17170.99290.14890.100*H11C0.38950.97540.02180.091*H11C0.39260.97540.02180.091*H11A0.23281.00840.0326 | H5A | 0.5130 (17) | 0.774 (2) | 0.1670 (9) | 0.049 (5)* | |
| C2 $0.09223 (18)$ $0.4295 (3)$ $0.18515 (9)$ $0.0616 (5)$ H2 0.1152 0.4707 0.2275 $0.074*$ C3 $-0.0371 (2)$ $0.3568 (3)$ $0.17039 (13)$ $0.0847 (7)$ H3 -0.1001 0.3499 0.2031 $0.102*$ C4 $-0.07241 (19)$ $0.2958 (3)$ $0.10887 (13)$ $0.0788 (6)$ H4 -0.1590 0.2474 0.0995 $0.095*$ C5 $0.02009 (18)$ $0.3061 (3)$ $0.06068 (10)$ $0.0631 (5)$ H5 -0.0038 0.2645 0.0185 $0.076*$ C6 $0.14894 (15)$ $0.3779 (2)$ $0.07445 (8)$ $0.0462 (4)$ H6 0.2111 0.3842 0.0414 $0.055*$ C7 $0.32751 (14)$ $0.51735 (18)$ $0.15342 (6)$ $0.0349 (3)$ H7 0.3268 0.5674 0.1978 $0.042*$ C8 $0.37089 (14)$ $0.5588 (18)$ $0.10615 (6)$ $0.0349 (3)$ H8 0.3817 0.6063 0.0630 $0.042*$ C9 $0.26314 (16)$ $0.8039 (2)$ $0.09599 (7)$ $0.0448 (4)$ H9 0.1749 0.7495 0.822 $0.0670 (5)$ H10A 0.3262 0.9619 0.1731 $0.100*$ H10B 0.2121 0.8312 0.1922 $0.100*$ H10C 0.1717 0.9929 0.1489 $0.100*$ H11B $0.3024 (2)$ $0.9215 (2)$ $0.04006 (8)$ $0.0606 (5)$ H11A 0.2328 1.0084 0.3256 $0.091*$ <td>C1</td> <td>0.18648 (14)</td> <td>0.44056 (18)</td> <td>0.13683 (7)</td> <td>0.0374 (3)</td> <td></td> | C1 | 0.18648 (14) | 0.44056 (18) | 0.13683 (7) | 0.0374 (3) | |
| H2 0.1152 0.4707 0.2275 $0.074*$ C3 -0.0371 (2) 0.3568 (3) 0.17039 (13) 0.0847 (7)H3 -0.1001 0.3499 0.2031 $0.102*$ C4 -0.07241 (19) 0.2958 (3) 0.10887 (13) 0.0788 (6)H4 -0.1590 0.2474 0.0995 $0.095*$ C5 0.02009 (18) 0.3061 (3) 0.06068 (10) 0.0331 (5)H5 -0.0038 0.2645 0.0185 $0.076*$ C6 0.14894 (15) 0.3779 (2) 0.07445 (8) 0.0462 (4)H6 0.2111 0.3842 0.0414 $0.055*$ C7 0.32751 (14) 0.51735 (18) 0.15342 (6) 0.0349 (3)H7 0.3268 0.5674 0.1978 $0.042*$ C8 0.37089 (14) 0.65989 (18) 0.10615 (6) 0.0349 (3)H8 0.817 0.6063 0.6630 $0.042*$ C9 0.26314 (16) 0.8039 (2) 0.9959 (7) 0.448 (4)H9 0.1749 0.7495 0.822 0.0670 (5)H10A 0.3262 0.9619 0.1731 $0.100*$ H10B 0.2121 0.8312 0.1922 $0.100*$ H10B 0.3024 (2) 0.9215 (2) 0.04006 (8) 0.6606 (5)H11A 0.3328 1.0084 0.0326 $0.091*$ H11B 0.3096 0.8550 0.0055 $0.091*$ H11B 0.3096 0.8556 (3) 0.12893 (10) 0.612 (5) <tr<< td=""><td>C2</td><td>0.09223 (18)</td><td>0.4295 (3)</td><td>0.18515 (9)</td><td>0.0616 (5)</td><td></td></tr<<> | C2 | 0.09223 (18) | 0.4295 (3) | 0.18515 (9) | 0.0616 (5) | |
| C3 $-0.0371(2)$ $0.3568(3)$ $0.17039(13)$ $0.0847(7)$ H3 -0.1001 0.3499 0.2031 $0.102*$ C4 $-0.07241(19)$ $0.2958(3)$ $0.10887(13)$ $0.0788(6)$ H4 -0.1590 0.2474 0.0995 $0.095*$ C5 $0.02009(18)$ $0.3061(3)$ $0.66068(10)$ $0.0631(5)$ H5 -0.0038 0.2645 0.0185 $0.076*$ C6 $0.14894(15)$ $0.3779(2)$ $0.07445(8)$ $0.0462(4)$ H6 0.2111 0.3842 0.0414 $0.055*$ C7 $0.32751(14)$ $0.51735(18)$ $0.15342(6)$ $0.0349(3)$ H7 0.3268 0.5674 0.1978 $0.042*$ C8 $0.37089(14)$ $0.65989(18)$ $0.1615(6)$ $0.0349(3)$ H8 0.3817 0.6063 0.0630 $0.042*$ C9 $0.26314(16)$ $0.8039(2)$ $0.09599(7)$ $0.448(4)$ H9 0.1749 7.495 0.0822 0.0574 C10 $0.2413(2)$ $0.9070(3)$ $0.15828(9)$ $0.100*$ H10R 0.3262 0.9619 0.1731 $0.100*$ H10B 0.2121 0.8312 0.1489 $0.100*$ C11 $0.3024(2)$ $0.9215(2)$ $0.4006(8)$ $0.6666(5)$ H11A 0.3285 0.9754 0.0218 $0.091*$ H11B 0.3096 0.8550 0.0005 $0.91*$ H11B $0.399(18)$ $0.7136(19)$ $0.9255(7)$ $0.418(3)$ C12 $0.61938(15)$ | H2 | 0.1152 | 0.4707 | 0.2275 | 0.074* | |
| H3-0.10010.34990.20310.102*C4-0.07241 (19)0.2958 (3)0.10887 (13)0.0788 (6)H4-0.15900.24740.09950.095*C50.02009 (18)0.3061 (3)0.06068 (10)0.0631 (5)H5-0.00380.26450.01850.076*C60.14894 (15)0.3779 (2)0.07445 (8)0.0462 (4)H60.21110.38420.04140.055*C70.32751 (14)0.51735 (18)0.15342 (6)0.0349 (3)H70.32680.56740.19780.042*C80.37089 (14)0.60630.06300.042*C90.26314 (16)0.8039 (2)0.09599 (7)0.0448 (4)H90.17490.74950.08220.054*C100.21210.83120.19220.100*H10A0.32620.96190.17310.100*H10B0.21210.83120.19220.100*H11A0.32381.00840.03260.091*C110.3024 (2)0.9215 (2)0.04006 (8)0.0606 (5)H11A0.32850.97540.05180.091*C130.74903 (18)0.73690.11550.091*H11C0.38950.97540.05180.091*H13A0.82770.73090.11150.092*H13A0.7493 (18)0.76470.17560.092*H13A0.7493 (18)0.76470.1766 (7)0.0412 (3)H13A0.7493 (| C3 | -0.0371 (2) | 0.3568 (3) | 0.17039 (13) | 0.0847 (7) | |
| C4 $-0.07241 (19)$ $0.2958 (3)$ $0.10887 (13)$ $0.0788 (6)$ H4 -0.1590 0.2474 0.0995 $0.095*$ C5 $0.02009 (18)$ $0.3061 (3)$ $0.06068 (10)$ $0.0631 (5)$ H5 -0.0038 0.2645 0.0185 $0.076*$ C6 $0.14894 (15)$ $0.3779 (2)$ $0.07445 (8)$ $0.0462 (4)$ H6 0.2111 0.3842 0.0414 $0.055*$ C7 $0.32751 (14)$ $0.51735 (18)$ $0.15342 (6)$ $0.3349 (3)$ H7 0.3268 0.5674 0.1978 $0.042*$ C8 $0.37089 (14)$ $0.65989 (18)$ $0.10615 (6)$ $0.0349 (3)$ H8 0.3817 0.0603 0.0630 $0.42*$ C9 $0.26314 (16)$ $0.8039 (2)$ $0.9599 (7)$ $0.4448 (4)$ H9 0.1749 0.7495 0.0822 $0.057*$ C10 $0.2413 (2)$ $0.9070 (3)$ $0.15828 (9)$ $0.0670 (5)$ H10A 0.3262 0.9619 0.1731 $0.100*$ H10B 0.2121 0.8312 0.1922 $0.100*$ H11A $0.324 (2)$ $0.9215 (2)$ $0.04006 (8)$ $0.0606 (5)$ H11A 0.3395 0.9754 0.0518 $0.091*$ C12 $0.61938 (15)$ $0.7136 (19)$ $0.9555 (7)$ $0.418 (3)$ C13 $0.7493 (18)$ 0.7647 $0.12893 (10)$ $0.612 (5)$ H13A 0.8277 0.7309 0.1115 $0.992*$ H13B $0.7493 (18)$ 0.7647 $0.1766 (7)$ < | Н3 | -0.1001 | 0.3499 | 0.2031 | 0.102* | |
| H4-0.15900.24740.09950.095*C50.02009 (18)0.3061 (3)0.06068 (10)0.0631 (5)H5-0.00380.26450.01850.076*C60.14894 (15)0.3779 (2)0.07445 (8)0.0462 (4)H60.21110.38420.04140.055*C70.32751 (14)0.51735 (18)0.15342 (6)0.0349 (3)H70.32680.56740.19780.042*C80.37089 (14)0.65989 (18)0.10615 (6)0.0349 (3)H80.38170.60630.06300.042*C90.26314 (16)0.8039 (2)0.09599 (7)0.0448 (4)H90.17490.74950.8220.0570 (5)H10A0.32620.90190.17310.100*H10B0.21210.83120.19220.100*H10C0.17170.99290.14890.100*H11B0.30960.85500.00050.091*H11B0.30960.85500.00050.091*H11B0.30960.8556 (3)0.1283 (10)0.612 (5)H13A0.82770.73090.11150.092*C120.61938 (15)0.76470.17560.092*H13B0.74930.76470.17560.092*H13B0.74930.76470.1766 (7)0.0412 (3)H13C0.75310.90740.12100.092*C140.49788 (15)0.3355 (19)0.10746 (7)0.0412 (3)H140.482 | C4 | -0.07241 (19) | 0.2958 (3) | 0.10887 (13) | 0.0788 (6) | |
| C5 0.02009 (18) 0.3061 (3) 0.06068 (10) 0.0631 (5) H5 -0.0038 0.2645 0.0185 0.076* C6 0.14894 (15) 0.3779 (2) 0.07445 (8) 0.0462 (4) H6 0.2111 0.3842 0.0414 0.055* C7 0.32751 (14) 0.51735 (18) 0.15342 (6) 0.0349 (3) H7 0.3268 0.5674 0.1978 0.042* C8 0.37089 (14) 0.65989 (18) 0.10615 (6) 0.0349 (3) H8 0.3817 0.6063 0.0630 0.042* C9 0.26314 (16) 0.8039 (2) 0.09599 (7) 0.0448 (4) H9 0.1749 0.7495 0.0822 0.054* C10 0.2413 (2) 0.9070 (3) 0.15828 (9) 0.0670 (5) H10A 0.3262 0.9619 0.1731 0.100* H10B 0.2121 0.8312 0.1922 0.100* C11 0.3024 (2) 0.9215 (2) 0.40406 (8) 0.6666 (5) | H4 | -0.1590 | 0.2474 | 0.0995 | 0.095* | |
| H5-0.00380.26450.01850.076*C60.14894 (15)0.3779 (2)0.07445 (8)0.0462 (4)H60.21110.38420.04140.055*C70.32751 (14)0.51735 (18)0.15342 (6)0.0349 (3)H70.32680.56740.19780.042*C80.37089 (14)0.65989 (18)0.10615 (6)0.0349 (3)H80.38170.60630.06300.042*C90.26314 (16)0.8039 (2)0.09599 (7)0.0448 (4)H90.17490.74950.08220.054*C100.2413 (2)0.9070 (3)0.15828 (9)0.0670 (5)H10A0.32620.96190.17310.100*H10B0.21210.83120.19220.100*H10C0.17170.99290.14890.100*C110.3024 (2)0.9215 (2)0.04006 (8)0.0666 (5)H11A0.23281.00840.03260.091*H11B0.30960.85500.00050.091*H11C0.38950.97540.05180.091*C120.61938 (15)0.71366 (19)0.09555 (7)0.0418 (3)C130.74903 (18)0.7856 (3)0.12893 (10)0.0612 (5)H13A0.82770.73090.11150.092*H13B0.74930.76470.17560.092*H13B0.74930.76470.12100.092*H13C0.75310.90740.12100.092*H13C< | C5 | 0.02009 (18) | 0.3061 (3) | 0.06068 (10) | 0.0631 (5) | |
| C60.14894 (15)0.3779 (2)0.07445 (8)0.0462 (4)H60.21110.38420.04140.055*C70.32751 (14)0.51735 (18)0.15342 (6)0.0349 (3)H70.32680.56740.19780.042*C80.37089 (14)0.65989 (18)0.10615 (6)0.0349 (3)H80.38170.60630.06300.042*C90.26314 (16)0.8039 (2)0.09599 (7)0.0448 (4)H90.17490.74950.08220.054*C100.2413 (2)0.9070 (3)0.15828 (9)0.0670 (5)H10A0.32620.96190.17310.100*H10B0.21210.83120.19220.100*H10C0.17170.99290.14890.100*H11A0.32381.00840.03260.091*H11B0.30960.85500.00050.091*H11B0.30960.85500.00050.091*H11C0.3895 (15)0.71366 (19)0.9555 (7)0.0418 (3)C130.74903 (18)0.7856 (3)0.12893 (10)0.612 (5)H13A0.82770.73090.11150.092*H13B0.74930.76470.17560.092*H13B0.74930.76470.17560.092*H13B0.74930.76470.12100.092*H13B0.74930.76470.12100.092*H13B0.74930.76470.17560.092*H13A0.4822 <td< td=""><td>Н5</td><td>-0.0038</td><td>0.2645</td><td>0.0185</td><td>0.076*</td><td></td></td<> | Н5 | -0.0038 | 0.2645 | 0.0185 | 0.076* | |
| H60.21110.38420.04140.055*C70.32751 (14)0.51735 (18)0.15342 (6)0.0349 (3)H70.32680.56740.19780.042*C80.37089 (14)0.65989 (18)0.10615 (6)0.0349 (3)H80.38170.60630.06300.042*C90.26314 (16)0.8039 (2)0.09599 (7)0.0448 (4)H90.17490.74950.08220.0574*C100.2413 (2)0.9070 (3)0.15828 (9)0.0670 (5)H10A0.32620.96190.17310.100*H10B0.21210.83120.19220.100*H10C0.17170.99290.14890.100*C110.3024 (2)0.9215 (2)0.04006 (8)0.6606 (5)H11A0.23281.00840.03260.091*H11B0.30960.85500.00050.091*H11C0.38950.97540.05180.091*C120.61938 (15)0.71366 (19)0.9555 (7)0.0418 (3)C130.74903 (18)0.7856 (3)0.12893 (10)0.612 (5)H13A0.82770.73090.11150.092*H13B0.74930.76470.17560.092*H13B0.74930.76470.17560.092*H13B0.74930.76470.12100.092*C140.49788 (15)0.30355 (19)0.10746 (7)0.412 (3)H140.48220.32640.6260.49* | C6 | 0.14894 (15) | 0.3779 (2) | 0.07445 (8) | 0.0462 (4) | |
| C70.32751 (14)0.51735 (18)0.15342 (6)0.0349 (3)H70.32680.56740.19780.042*C80.37089 (14)0.65989 (18)0.10615 (6)0.0349 (3)H80.38170.60630.06300.042*C90.26314 (16)0.8039 (2)0.09599 (7)0.0448 (4)H90.17490.74950.08220.054*C100.2413 (2)0.9070 (3)0.15828 (9)0.0670 (5)H10A0.32620.96190.17310.100*H10B0.21210.83120.19220.100*H10C0.17170.99290.14890.100*C110.3024 (2)0.9215 (2)0.04006 (8)0.06606 (5)H11A0.23281.00840.03260.091*H11C0.38950.97540.05180.091*C120.61938 (15)0.71366 (19)0.09555 (7)0.0418 (3)C130.74903 (18)0.7856 (3)0.12893 (10)0.0612 (5)H13A0.82770.73090.11150.092*H13B0.74930.76470.17560.092*H13B0.74930.90740.12100.092*H13C0.75310.90740.12100.092*H140.48220.32640.06260.049* | H6 | 0.2111 | 0.3842 | 0.0414 | 0.055* | |
| H70.32680.56740.19780.042*C80.37089 (14)0.65989 (18)0.10615 (6)0.0349 (3)H80.38170.60630.06300.042*C90.26314 (16)0.8039 (2)0.09599 (7)0.0448 (4)H90.17490.74950.08220.054*C100.2413 (2)0.9070 (3)0.15828 (9)0.0670 (5)H10A0.32620.96190.17310.100*H10B0.21210.83120.19220.100*H10C0.17170.99290.14890.100*C110.3024 (2)0.9215 (2)0.04006 (8)0.0606 (5)H11A0.23281.00840.03260.091*H11B0.30960.85500.005180.091*C120.61938 (15)0.71366 (19)0.09555 (7)0.0418 (3)C130.74903 (18)0.7856 (3)0.12893 (10)0.0612 (5)H13B0.74930.76470.17560.092*H13B0.74930.76470.17560.092*H13C0.75310.90740.12100.092*C140.49788 (15)0.30355 (19)0.10746 (7)0.0412 (3)H140.48220.32640.06260.049* | C7 | 0.32751 (14) | 0.51735 (18) | 0.15342 (6) | 0.0349 (3) | |
| C80.37089 (14)0.65989 (18)0.10615 (6)0.0349 (3)H80.38170.60630.06300.042*C90.26314 (16)0.8039 (2)0.09599 (7)0.0448 (4)H90.17490.74950.08220.054*C100.2413 (2)0.9070 (3)0.15828 (9)0.0670 (5)H10A0.32620.96190.17310.100*H10B0.21210.83120.19220.100*H10C0.17170.99290.14890.100*C110.3024 (2)0.9215 (2)0.04006 (8)0.0660 (5)H11A0.23281.00840.03260.091*H11B0.30960.85500.00050.091*H11C0.38950.97540.05180.091*C120.61938 (15)0.71366 (19)0.09555 (7)0.0418 (3)C130.74903 (18)0.7856 (3)0.12893 (10)0.0612 (5)H13A0.82770.73090.11150.092*H13B0.74930.76470.17560.092*H13C0.75310.90740.12100.092*C140.49788 (15)0.30355 (19)0.10746 (7)0.0412 (3)H140.48220.32640.06260.049* | H7 | 0.3268 | 0.5674 | 0.1978 | 0.042* | |
| H80.38170.60630.06300.042*C90.26314 (16)0.8039 (2)0.09599 (7)0.0448 (4)H90.17490.74950.08220.054*C100.2413 (2)0.9070 (3)0.15828 (9)0.0670 (5)H10A0.32620.96190.17310.100*H10B0.21210.83120.19220.100*H10C0.17170.99290.14890.100*C110.3024 (2)0.9215 (2)0.04006 (8)0.0660 (5)H11A0.23281.00840.03260.091*H11B0.30960.85500.00050.091*H11C0.38950.97540.05180.091*C120.61938 (15)0.71366 (19)0.09555 (7)0.0418 (3)C130.74903 (18)0.7856 (3)0.12893 (10)0.0612 (5)H13A0.82770.73090.11150.092*H13B0.74930.90740.12100.092*H13C0.75310.90740.12100.092*C140.49220.32640.06260.049* | C8 | 0.37089 (14) | 0.65989 (18) | 0.10615 (6) | 0.0349 (3) | |
| C90.26314 (16)0.8039 (2)0.09599 (7)0.0448 (4)H90.17490.74950.08220.054*C100.2413 (2)0.9070 (3)0.15828 (9)0.0670 (5)H10A0.32620.96190.17310.100*H10B0.21210.83120.19220.100*H10C0.17170.99290.14890.100*C110.3024 (2)0.9215 (2)0.04006 (8)0.06606 (5)H11A0.23281.00840.03260.091*H11B0.30960.85500.00050.091*H11C0.38950.97540.05180.091*C120.61938 (15)0.71366 (19)0.9555 (7)0.0418 (3)C130.74903 (18)0.7856 (3)0.12893 (10)0.0612 (5)H13A0.82770.73090.11150.092*H13B0.74930.76470.17560.092*H13C0.75310.90740.12100.092*C140.49788 (15)0.30355 (19)0.10746 (7)0.0412 (3)H140.48220.32640.06260.049* | H8 | 0.3817 | 0.6063 | 0.0630 | 0.042* | |
| H90.17490.74950.08220.054*C100.2413 (2)0.9070 (3)0.15828 (9)0.0670 (5)H10A0.32620.96190.17310.100*H10B0.21210.83120.19220.100*H10C0.17170.99290.14890.100*C110.3024 (2)0.9215 (2)0.04006 (8)0.0606 (5)H11A0.23281.00840.03260.091*H11B0.30960.85500.00050.091*H11C0.38950.97540.05180.091*C120.61938 (15)0.71366 (19)0.09555 (7)0.0418 (3)C130.74903 (18)0.7856 (3)0.12893 (10)0.0612 (5)H13A0.82770.73090.11150.092*H13B0.74930.76470.17560.092*H13C0.75310.90740.12100.092*C140.49788 (15)0.30355 (19)0.10746 (7)0.0412 (3)H140.48220.32640.06260.049* | C9 | 0.26314 (16) | 0.8039 (2) | 0.09599 (7) | 0.0448 (4) | |
| C100.2413 (2)0.9070 (3)0.15828 (9)0.0670 (5)H10A0.32620.96190.17310.100*H10B0.21210.83120.19220.100*H10C0.17170.99290.14890.100*C110.3024 (2)0.9215 (2)0.04006 (8)0.0606 (5)H11A0.23281.00840.03260.091*H11B0.30960.85500.00050.091*H11C0.38950.97540.05180.091*C120.61938 (15)0.71366 (19)0.09555 (7)0.0418 (3)C130.74903 (18)0.7856 (3)0.12893 (10)0.6612 (5)H13B0.74930.76470.17560.092*H13B0.74930.90740.12100.092*H13C0.75310.90740.10746 (7)0.0412 (3)H140.48220.32640.06260.049* | H9 | 0.1749 | 0.7495 | 0.0822 | 0.054* | |
| H10A0.32620.96190.17310.100*H10B0.21210.83120.19220.100*H10C0.17170.99290.14890.100*C110.3024 (2)0.9215 (2)0.04006 (8)0.0606 (5)H11A0.23281.00840.03260.091*H11B0.30960.85500.00050.091*H11C0.38950.97540.05180.091*C120.61938 (15)0.71366 (19)0.09555 (7)0.0418 (3)C130.74903 (18)0.7856 (3)0.12893 (10)0.0612 (5)H13B0.74930.76470.17560.092*H13C0.75310.90740.12100.092*C140.49788 (15)0.30355 (19)0.10746 (7)0.0412 (3)H140.48220.32640.06260.049* | C10 | 0.2413 (2) | 0.9070 (3) | 0.15828 (9) | 0.0670 (5) | |
| H10B0.21210.83120.19220.100*H10C0.17170.99290.14890.100*C110.3024 (2)0.9215 (2)0.04006 (8)0.0606 (5)H11A0.23281.00840.03260.091*H11B0.30960.85500.00050.091*H11C0.38950.97540.05180.091*C120.61938 (15)0.71366 (19)0.09555 (7)0.0418 (3)C130.74903 (18)0.7856 (3)0.12893 (10)0.0612 (5)H13A0.82770.73090.11150.092*H13B0.74930.76470.17560.092*H13C0.75310.90740.12100.092*C140.49788 (15)0.30355 (19)0.10746 (7)0.0412 (3)H140.48220.32640.06260.049* | H10A | 0.3262 | 0.9619 | 0.1731 | 0.100* | |
| H10C0.17170.99290.14890.100*C110.3024 (2)0.9215 (2)0.04006 (8)0.0606 (5)H11A0.23281.00840.03260.091*H11B0.30960.85500.00050.091*H11C0.38950.97540.05180.091*C120.61938 (15)0.71366 (19)0.09555 (7)0.0418 (3)C130.74903 (18)0.7856 (3)0.12893 (10)0.0612 (5)H13A0.82770.73090.11150.092*H13B0.74930.76470.17560.092*H13C0.75310.90740.12100.092*C140.49788 (15)0.30355 (19)0.10746 (7)0.0412 (3)H140.48220.32640.06260.049* | H10B | 0.2121 | 0.8312 | 0.1922 | 0.100* | |
| C110.3024 (2)0.9215 (2)0.04006 (8)0.0606 (5)H11A0.23281.00840.03260.091*H11B0.30960.85500.00050.091*H11C0.38950.97540.05180.091*C120.61938 (15)0.71366 (19)0.09555 (7)0.0418 (3)C130.74903 (18)0.7856 (3)0.12893 (10)0.0612 (5)H13A0.82770.73090.11150.092*H13B0.74930.76470.17560.092*H13C0.75310.90740.12100.092*C140.49788 (15)0.30355 (19)0.10746 (7)0.0412 (3)H140.48220.32640.06260.049* | H10C | 0.1717 | 0.9929 | 0.1489 | 0.100* | |
| H11A0.23281.00840.03260.091*H11B0.30960.85500.00050.091*H11C0.38950.97540.05180.091*C120.61938 (15)0.71366 (19)0.09555 (7)0.0418 (3)C130.74903 (18)0.7856 (3)0.12893 (10)0.0612 (5)H13A0.82770.73090.11150.092*H13B0.74930.76470.17560.092*H13C0.75310.90740.12100.092*C140.49788 (15)0.30355 (19)0.10746 (7)0.0412 (3)H140.48220.32640.06260.049* | C11 | 0.3024 (2) | 0.9215 (2) | 0.04006 (8) | 0.0606 (5) | |
| H11B0.30960.85500.00050.091*H11C0.38950.97540.05180.091*C120.61938 (15)0.71366 (19)0.09555 (7)0.0418 (3)C130.74903 (18)0.7856 (3)0.12893 (10)0.0612 (5)H13A0.82770.73090.11150.092*H13B0.74930.76470.17560.092*H13C0.75310.90740.12100.092*C140.49788 (15)0.30355 (19)0.10746 (7)0.0412 (3)H140.48220.32640.06260.049* | H11A | 0.2328 | 1.0084 | 0.0326 | 0.091* | |
| H11C0.38950.97540.05180.091*C120.61938 (15)0.71366 (19)0.09555 (7)0.0418 (3)C130.74903 (18)0.7856 (3)0.12893 (10)0.0612 (5)H13A0.82770.73090.11150.092*H13B0.74930.76470.17560.092*H13C0.75310.90740.12100.092*C140.49788 (15)0.30355 (19)0.10746 (7)0.0412 (3)H140.48220.32640.06260.049* | H11B | 0.3096 | 0.8550 | 0.0005 | 0.091* | |
| C120.61938 (15)0.71366 (19)0.09555 (7)0.0418 (3)C130.74903 (18)0.7856 (3)0.12893 (10)0.0612 (5)H13A0.82770.73090.11150.092*H13B0.74930.76470.17560.092*H13C0.75310.90740.12100.092*C140.49788 (15)0.30355 (19)0.10746 (7)0.0412 (3)H140.48220.32640.06260.049* | H11C | 0.3895 | 0.9754 | 0.0518 | 0.091* | |
| C130.74903 (18)0.7856 (3)0.12893 (10)0.0612 (5)H13A0.82770.73090.11150.092*H13B0.74930.76470.17560.092*H13C0.75310.90740.12100.092*C140.49788 (15)0.30355 (19)0.10746 (7)0.0412 (3)H140.48220.32640.06260.049* | C12 | 0.61938 (15) | 0.71366 (19) | 0.09555 (7) | 0.0418 (3) | |
| H13A0.82770.73090.11150.092*H13B0.74930.76470.17560.092*H13C0.75310.90740.12100.092*C140.49788 (15)0.30355 (19)0.10746 (7)0.0412 (3)H140.48220.32640.06260.049* | C13 | 0.74903 (18) | 0.7856 (3) | 0.12893 (10) | 0.0612 (5) | |
| H13B0.74930.76470.17560.092*H13C0.75310.90740.12100.092*C140.49788 (15)0.30355 (19)0.10746 (7)0.0412 (3)H140.48220.32640.06260.049* | H13A | 0.8277 | 0.7309 | 0.1115 | 0.092* | |
| H13C0.75310.90740.12100.092*C140.49788 (15)0.30355 (19)0.10746 (7)0.0412 (3)H140.48220.32640.06260.049* | H13B | 0.7493 | 0.7647 | 0.1756 | 0.092* | |
| C140.49788 (15)0.30355 (19)0.10746 (7)0.0412 (3)H140.48220.32640.06260.049* | H13C | 0.7531 | 0.9074 | 0.1210 | 0.092* | |
| H14 0.4822 0.3264 0.0626 0.049* | C14 | 0.49788 (15) | 0.30355 (19) | 0.10746 (7) | 0.0412 (3) | |
| | H14 | 0.4822 | 0.3264 | 0.0626 | 0.049* | |

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

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|-------------|--------------|
| 01 | 0.0576 (7) | 0.0833 (9) | 0.0399 (6) | -0.0092 (6) | 0.0106 (5) | -0.0082 (6) |
| N1 | 0.0361 (6) | 0.0374 (6) | 0.0285 (5) | -0.0026 (5) | -0.0029 (4) | 0.0043 (5) |
| N2 | 0.0667 (9) | 0.0659 (10) | 0.0332 (7) | 0.0124 (8) | -0.0060 (6) | 0.0102 (6) |
| N3 | 0.0647 (9) | 0.0653 (10) | 0.0501 (8) | 0.0157 (8) | -0.0092 (7) | 0.0129 (7) |
| N4 | 0.0438 (7) | 0.0479 (8) | 0.0530 (8) | 0.0046 (6) | -0.0004 (6) | 0.0068 (6) |
| N5 | 0.0420 (7) | 0.0423 (7) | 0.0318 (6) | -0.0075 (5) | -0.0008(5) | -0.0065 (5) |
| C1 | 0.0350 (7) | 0.0378 (8) | 0.0399 (7) | 0.0017 (6) | 0.0054 (5) | 0.0063 (6) |
| C2 | 0.0551 (10) | 0.0821 (14) | 0.0493 (9) | -0.0016 (9) | 0.0179 (8) | 0.0044 (9) |
| C3 | 0.0517 (11) | 0.1155 (19) | 0.0907 (16) | -0.0091 (12) | 0.0343 (11) | 0.0137 (14) |
| C4 | 0.0398 (10) | 0.0940 (16) | 0.1027 (17) | -0.0163 (10) | 0.0056 (10) | 0.0085 (14) |
| C5 | 0.0450 (9) | 0.0713 (13) | 0.0715 (12) | -0.0107 (9) | -0.0085 (8) | -0.0026 (10) |
| C6 | 0.0370 (7) | 0.0551 (9) | 0.0464 (8) | -0.0064 (7) | 0.0027 (6) | -0.0019 (7) |
| C7 | 0.0387 (7) | 0.0390 (7) | 0.0270 (6) | 0.0011 (6) | 0.0016 (5) | -0.0017 (5) |
| C8 | 0.0386 (7) | 0.0351 (7) | 0.0306 (6) | -0.0035 (6) | -0.0009(5) | -0.0012 (5) |
| C9 | 0.0461 (8) | 0.0410 (8) | 0.0465 (8) | 0.0017 (7) | -0.0036 (6) | 0.0025 (6) |
| C10 | 0.0816 (13) | 0.0610 (12) | 0.0592 (11) | 0.0248 (10) | 0.0116 (9) | -0.0017 (9) |
| C11 | 0.0816 (13) | 0.0461 (10) | 0.0534 (10) | 0.0048 (9) | -0.0025 (9) | 0.0108 (8) |
| C12 | 0.0440 (8) | 0.0414 (8) | 0.0396 (8) | -0.0044 (7) | 0.0000 (6) | 0.0053 (6) |
| C13 | 0.0458 (9) | 0.0648 (12) | 0.0720 (12) | -0.0081 (8) | -0.0040 (8) | -0.0034 (9) |
| C14 | 0.0436 (8) | 0.0442 (8) | 0.0356 (7) | 0.0023 (6) | 0.0014 (6) | 0.0030 (6) |

Atomic displacement parameters $(Å^2)$

Geometric parameters (Å, °)

| 01—C12 | 1.2221 (18) | С5—Н5 | 0.9300 |
|-----------|-------------|----------|-------------|
| N1-C14 | 1.3276 (18) | С6—Н6 | 0.9300 |
| N1—N2 | 1.3413 (16) | C7—C8 | 1.5392 (19) |
| N1—C7 | 1.4784 (18) | С7—Н7 | 0.9800 |
| N2—N3 | 1.295 (2) | C8—C9 | 1.536 (2) |
| N3—N4 | 1.3434 (19) | C8—H8 | 0.9800 |
| N4-C14 | 1.3079 (19) | C9—C10 | 1.520 (2) |
| N5-C12 | 1.3420 (19) | C9—C11 | 1.522 (2) |
| N5—C8 | 1.4562 (17) | С9—Н9 | 0.9800 |
| N5—H5A | 0.844 (18) | C10—H10A | 0.9600 |
| C1—C6 | 1.382 (2) | C10—H10B | 0.9600 |
| C1—C2 | 1.383 (2) | C10—H10C | 0.9600 |
| C1—C7 | 1.5120 (19) | C11—H11A | 0.9600 |
| С2—С3 | 1.392 (3) | C11—H11B | 0.9600 |
| С2—Н2 | 0.9300 | C11—H11C | 0.9600 |
| С3—С4 | 1.358 (3) | C12—C13 | 1.500 (2) |
| С3—Н3 | 0.9300 | C13—H13A | 0.9600 |
| C4—C5 | 1.368 (3) | C13—H13B | 0.9600 |
| C4—H4 | 0.9300 | C13—H13C | 0.9600 |
| C5—C6 | 1.382 (2) | C14—H14 | 0.9300 |
| C14—N1—N2 | 107.28 (12) | C9—C8—C7 | 113.40 (11) |
| | | | |

| C14—N1—C7 | 131.43 (11) | N5—C8—H8 | 107.4 |
|---------------------|--------------|---------------|--------------|
| N2—N1—C7 | 121.30 (11) | С9—С8—Н8 | 107.4 |
| N3—N2—N1 | 106.48 (12) | С7—С8—Н8 | 107.4 |
| N2—N3—N4 | 111.16 (12) | C10—C9—C11 | 110.85 (15) |
| C14—N4—N3 | 104.96 (13) | C10—C9—C8 | 113.59 (13) |
| C12—N5—C8 | 123.88 (12) | C11—C9—C8 | 109.73 (13) |
| C12—N5—H5A | 117.7 (11) | С10—С9—Н9 | 107.5 |
| C8—N5—H5A | 118.4 (11) | С11—С9—Н9 | 107.5 |
| C6—C1—C2 | 118.47 (14) | С8—С9—Н9 | 107.5 |
| C6—C1—C7 | 121.79 (12) | C9—C10—H10A | 109.5 |
| C2—C1—C7 | 119.73 (14) | C9—C10—H10B | 109.5 |
| C1—C2—C3 | 119.98 (18) | H10A-C10-H10B | 109.5 |
| C1—C2—H2 | 120.0 | C9—C10—H10C | 109.5 |
| С3—С2—Н2 | 120.0 | H10A-C10-H10C | 109.5 |
| C4—C3—C2 | 120.85 (17) | H10B—C10—H10C | 109.5 |
| С4—С3—Н3 | 119.6 | C9—C11—H11A | 109.5 |
| С2—С3—Н3 | 119.6 | C9—C11—H11B | 109.5 |
| $C_{3}-C_{4}-C_{5}$ | 119.66 (18) | H11A—C11—H11B | 109.5 |
| C3—C4—H4 | 120.2 | C9—C11—H11C | 109.5 |
| C5—C4—H4 | 120.2 | H11A—C11—H11C | 109.5 |
| C4—C5—C6 | 120.27 (19) | H11B—C11—H11C | 109.5 |
| C4—C5—H5 | 119.9 | 01—C12—N5 | 122.22 (14) |
| С6—С5—Н5 | 119.9 | O1—C12—C13 | 121.92 (14) |
| C5—C6—C1 | 120.77 (15) | N5—C12—C13 | 115.85 (14) |
| С5—С6—Н6 | 119.6 | С12—С13—Н13А | 109.5 |
| C1—C6—H6 | 119.6 | С12—С13—Н13В | 109.5 |
| N1—C7—C1 | 110.29 (11) | H13A—C13—H13B | 109.5 |
| N1—C7—C8 | 108.27 (10) | С12—С13—Н13С | 109.5 |
| C1—C7—C8 | 115.06 (11) | H13A—C13—H13C | 109.5 |
| N1—C7—H7 | 107.6 | H13B—C13—H13C | 109.5 |
| С1—С7—Н7 | 107.6 | N4—C14—N1 | 110.12 (13) |
| С8—С7—Н7 | 107.6 | N4—C14—H14 | 124.9 |
| N5—C8—C9 | 112.30 (12) | N1—C14—H14 | 124.9 |
| N5—C8—C7 | 108.76 (11) | | |
| | () | | |
| C14—N1—N2—N3 | 0.25 (17) | C6—C1—C7—C8 | 52.19 (19) |
| C7—N1—N2—N3 | -179.60 (13) | C2—C1—C7—C8 | -128.80 (15) |
| N1—N2—N3—N4 | -0.4 (2) | C12—N5—C8—C9 | -116.60 (15) |
| N2—N3—N4—C14 | 0.3 (2) | C12—N5—C8—C7 | 117.06 (14) |
| C6—C1—C2—C3 | -0.1 (3) | N1—C7—C8—N5 | -58.28 (13) |
| C7—C1—C2—C3 | -179.13 (18) | C1—C7—C8—N5 | 177.83 (11) |
| C1—C2—C3—C4 | 0.1 (4) | N1—C7—C8—C9 | 176.01 (11) |
| C2—C3—C4—C5 | -0.1 (4) | C1—C7—C8—C9 | 52.12 (16) |
| C3—C4—C5—C6 | 0.1 (4) | N5-C8-C9-C10 | -58.69 (17) |
| C4—C5—C6—C1 | 0.0 (3) | C7—C8—C9—C10 | 65.11 (17) |
| C2—C1—C6—C5 | 0.1 (3) | N5-C8-C9-C11 | 66.00 (16) |
| C7—C1—C6—C5 | 179.09 (15) | C7—C8—C9—C11 | -170.20 (12) |
| C14—N1—C7—C1 | 80.54 (17) | C8—N5—C12—O1 | 0.1 (2) |
| | × · · / | - | / |

| N2-N1-C7-C1 | -99.66 (14) | C8—N5—C12—C13 | -178.70 (14) |
|--------------|-------------|---------------|--------------|
| C14—N1—C7—C8 | -46.17 (18) | N3—N4—C14—N1 | -0.15 (18) |
| N2—N1—C7—C8 | 133.64 (13) | N2—N1—C14—N4 | -0.06 (17) |
| C6—C1—C7—N1 | -70.63 (16) | C7—N1—C14—N4 | 179.77 (13) |
| C2-C1-C7-N1 | 108.39 (16) | | |

Hydrogen-bond geometry (Å, °)

| D—H···A | D—H | H···A | D····A | <i>D</i> —H··· <i>A</i> |
|--------------------------|------------|------------|-------------|-------------------------|
| N5—H5A···N2 ⁱ | 0.844 (18) | 2.452 (18) | 3.2579 (17) | 160.0 (15) |
| C6—H6…O1 ⁱⁱ | 0.93 | 2.43 | 3.356 (2) | 171 |
| C7—H7····N3 ⁱ | 0.98 | 2.48 | 3.4055 (19) | 157 |
| C14—H14…O1 ⁱⁱ | 0.93 | 2.27 | 3.1728 (19) | 163 |

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