Crystal structure of the complex of 2,4,6-triethyl-1,3,5-tris[(4-methyl-1H-indazol-1-yl)methyl]benzene with NH₄PF₆

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The complex of 2,4,6-triethyl-1,3,5-tris[(4-methyl-1H-indazol-1-yl)methyl]benzene with ammonium hexafluorophosphate, C₃₉H₄₂N₆/CH₄NH₄⁺/C₁PF₆⁻, crystallizes in the monoclinic space group P₂₁ with two molecules of the receptor, two NH₄⁺ and two PF₆⁻ ions in the asymmetric unit. In each of the complexes the ammonium ion resides in the cavity of the receptor molecule and is fixed in its position by three N—H···N bonds, while the remaining hydrogen atom of the cation acts as a bifurcated binding site for N—H···F bonding to the counteranion. The crystal is composed of one-dimensional supramolecular aggregates extending along the a-axis direction.

1. Chemical context

The development of efficient artificial receptors that exhibit high selectivity for ammonium versus potassium ions is of great interest (Bühlmann et al., 1998; Chin et al., 1999; Späth & König, 2010; Pazik & Skwierawska, 2014; Jonah et al., 2017; Schulze et al., 2018). Both acyclic and macrocyclic receptors have been designed to achieve this goal. Tripodal and hexa-podal benzene derivatives bearing pyrazolyl or indazolyl groups have proven to be promising as receptors for NH₄⁺ (Chin et al., 1999, 2002; Koch et al., 2015; Jonah et al., 2017; Schulze et al., 2018). The ability of these compounds to act as ammonium receptors has been examined both in solution and in the crystalline state. Structural variations are to be used to develop receptor molecules that exhibit a more pronounced selectivity. As part of our studies on structure–binding affinity relationships, we have synthesized various acyclic molecules and investigated their binding properties. In this work we describe the crystal structure of a complex between NH₄PF₆ and a tripodal benzene derivative bearing 4-methyl-indazol-1-yl groups.
2. Structural commentary

Crystallization from a mixture of the title compound and NH₄PF₆ in ethanol yields colourless prisms of the monoclinic space group P2₁ with two molecules of the receptor, two NH₄⁺ ions and two PF₆⁻ ions in the asymmetric unit. These components are connected to form complexes of the structures shown in Fig. 1. In each of them, the NH₄⁺ ion resides in a cavity created by the indazolyl groups of the receptor and is held in its position by three N—H⋯N bonds [d(H⋯N) 2.01 (2)–2.10 (4) Å], involving the nitrogen atoms designated N2, N4, N6 and N2A, N4A, N6A. The remaining H atom of the ammonium acts as a bifurcated binding site for N—H⋯F bonding with the counter-ion. The conformational difference between the receptor molecules is seen in the orientation of the three ethyl groups, leading to an ab’ab’ab’ (complex I) and an ab’aa’ab’ (complex II) (a = above, b = below, a’b’ = ethyl; see Koch et al., 2017; Schulze et al., 2017) of substituents with respect to the plane of the central arene ring (Fig. 2). The dihedral angles between the planes of the indazole units are 67.8 (1), 8.1 (2), 72.6 (1)° for complex I and 62.0 (1), 6.9 (2), 65.4 (1)° for complex II.

3. Supramolecular features

The crystal is composed of one-dimensional supramolecular aggregates of C—H⋯F-bonded ammonium complexes [d(H⋯F) 2.33–2.52 Å; Table 1] extending in the a-axis direction. The packing is shown in Fig. 3. Multiple π–π arene contacts connect these aggregates into a three-dimensional network. For the analysis of this type of interactions, the PLATON program (Spek, 2020) was used. The centroid–centroid distances between the interacting indazole units range from 3.776 (4) to 4.257 (4) Å with shifts of 1.154–1.830 Å.

4. Database survey

A search in the Cambridge Structural Database (CSD, Version 5.40, updated February 2019; Groom et al., 2016) for ammonium complexes of 1,3,5-substituted 2,4,6-trialkylbenzenes bearing pyrazolyl or indazolyl units gave eight hits, all of which contain complexes with NH₄PF₆. The complexes of 1,3,5-tris[(3,5-dimethyl-1H-pyrazol-1-yl)methyl]-2,4,6-triethylbenzene (CUKTUX; Chin et al., 1999), 1,3,5-tris[(4-bromo-3,5-dimethyl-1H-pyrazol-1-yl)methyl]-2,4,6-triethylbenzene (UFOHOM; Chin et al., 2002), 1,3,5-tris[(1H-pyrazol-1-yl)methyl]-2,4,6-trimethylbenzene (QIFFAP; Schulze et al., 2018), 1,3,5-tris[(3,5-dimethyl-1H-pyrazol-1-yl)methyl]-2,4,6-trimethylbenzene (QIDTOP; Schulze et al., 2018) and 1,3,5-tris[(4-
bromo-3,5-dimethyl-1H-pyrazol-1-yl)methyl]-2,4,6-trimethylbenzene (QIDTUV; Schulze et al., 2018) have the most similar structures to that of the title complex. In the crystal structure of the complex formed by 1,3,5-tris[(4-bromo-3,5-dimethyl-1H-pyrazol-1-yl)methyl]-2,4,6-triethylbenzene (QIDVOR; Schulze et al., 2018), which also contains acetanilide molecules, the complex lacks NH...F7...P6 interactions. Instead, one of the solvent molecules is connected to the cation via N—H···N bonding whereas the PF6− ion is coordinated to the receptor and the solvent molecules. In the crystal of the complex of 1,3,5-tris[(3,5-diphenyl-1H-pyrazol-1-yl)methyl]-2,4,6-triethylbenzene (XEBEX; Jonah et al., 2017) the steric demand of the phenyl groups attached to the pyrazole rings prevents cation-anion interactions. In the case of the complex of 1,3,5-tris[(1H-indazol-1-yl)methyl]-2,4,6-triethylbenzene (QIDVAD; Schulze et al., 2018), the asymmetric unit contains four receptor molecules, four NH4PF6, one water and two methanol molecules. As a result, complexes are formed, the structures of which differ strongly from that of the title complex.

5. Synthesis and crystallization

To a solution of 4-methyl-1H-indazole (500 mg, 3.78 mmol) in dimethylformamide (9.0 mL) sodium hydroxide (152 mg, 3.78 mmol) was added and the suspension was stirred at room temperature for 30 minutes. Then 1,3,5-tris(bromomethyl)-2,4,6-triethylbenzene (418 mg, 0.95 mmol) was added and the mixture stirred at 343 K for 24 h. After cooling to room temperature, the reaction mixture was poured into ice–water (55 mL). The precipitate was filtered off, washed with a little ice–water and dried under reduced pressure. The crude mixture, containing the desired product as well as two other triethylbenzene derivatives and the unreacted 4-methyl-1H-indazole, was separated chromatographically. The first flash chromatography (SiO2; gradient, hexane/ethyl acetate 4:1 to 3:2, v/v) allowed the isolation of the by-products 2,4,6-triethyl-1,3-bis[(4-methyl-1H-indazol-1-yl)methyl]-5[(4-methyl-2H-indazol-2-yl)methyl]benzene and 2,4,6-triethyl-1,3-bis[(4-methyl-2H-indazol-2-yl)methyl]-5[(4-methyl-1H-indazol-1-yl)methyl]benzene, while the second one (SiO2; gradient, toluene/ethyl acetate 16:1 to 4:1, v/v) enabled the removal of 4-methyl-1H-indazole. After crystallization from hexane/ethyl acetate (2:1, v/v) the title compound was obtained as colourless crystals (110 mg, 20%); m.p. 427–429 K. 1H NMR (500 MHz, CDCl3, ppm) δ = 0.80 (t, J = 7.5 Hz, 9H), 2.58 (s, 9H), 2.89 (q, J = 7.5 Hz, 6H), 5.63 (s, 6H), 6.87 (dt, J = 7.0/1.0 Hz, 3H), 7.03 (dd, J = 8.5/1.0 Hz, 3H), 7.12 (dd, J = 8.5/7.0 Hz, 3H), 8.01 (d, J = 1.0 Hz, 3H). 13C NMR (125 MHz, CDCl3, ppm) δ = 14.7, 18.6, 23.8, 47.6, 107.0, 120.5, 124.8, 126.5, 130.6, 131.4, 132.0, 139.6, 145.7.

Table 1

| Crystal data | C29H42N6PF6 | Monoclinic, P21 |
| Temperature (K) | 123 | 11.1251 (11), 31.590 (2), 11.1558 (11) |
| a, b, c (Å) | 11.251 (11), 31.590 (2), 11.1558 (11) | 92.751 (8), 3916.1 (6) |
| Microscopy type | Mo Kα | 0.14 |
| Crystal size (mm) | 0.28 × 0.25 × 0.18 | |

Table 2

| Experimental details. |
| Crystal data | C29H42N6PF6 | Monoclinic, P21 |
| Temperature (K) | 123 | 11.1251 (11), 31.590 (2), 11.1558 (11) |
| a, b, c (Å) | 11.251 (11), 31.590 (2), 11.1558 (11) | 92.751 (8), 3916.1 (6) |
| Microscopy type | Mo Kα | 0.14 |
| Crystal size (mm) | 0.28 × 0.25 × 0.18 | |
6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The hydrogen atoms were positioned geometrically and refined isotropically using the riding model with C—H = 0.95–0.99 Å and $U_{eq}(H) = 1.2$ or $1.5U_{eq}(C)$. The hydrogen atoms of the ammonium ions were located in a difference-Fourier map and the N—H bond lengths refined to a target value of 0.90 Å. The crystal studied was refined as a two-component twin.

Acknowledgements

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Computing details
Data collection: X-AREA (Stoe & Cie, 2002); cell refinement: X-AREA (Stoe & Cie, 2002); data reduction: X-RED (Stoe & Cie, 2002); program(s) used to solve structure: SHELXT2018/3 (Sheldrick, 2015a); program(s) used to refine structure: SHELXL2018/3 (Sheldrick, 2015b); molecular graphics: ORTEP-3 for Windows (Farrugia, 2012).

2,4,6-Triethyl-1,3,5-tris[(4-methyl-1H-indazol-1-yl)methyl]benzene–

Crystal data

| C$_{39}$H$_{42}$N$_6$·NH$_4^+$·PF$_6^-$ | F(000) = 1592 |
|--------------------------------|---------------|
| M$_r$ = 757.80 |
| Monoclinic, $P$2$_1$ |
| $a$ = 11.1251 (11) Å |
| $b$ = 31.590 (2) Å |
| $c$ = 11.1558 (11) Å |
| $\beta$ = 92.751 (8)° |
| $V$ = 3916.1 (6) Å$^3$ |
| $Z$ = 4 |
| $\mu$ = 0.14 mm$^{-1}$ |
| $D_x$ = 1.285 Mg m$^{-3}$ |
| Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å |
| Cell parameters from 19655 reflections |
| $\theta$ = 2.0–22.5° |
| $\mu$ = 0.14 mm$^{-1}$ |
| $T$ = 123 K |
| Irregular, colorless |
| 0.28 x 0.25 x 0.18 mm |

Data collection

Stoe IPDS 2T diffractometer
Radiation source: sealed X-ray tube, 12 x 0.4 mm-long-focus
Plane graphite monochromator
Detector resolution: 6.67 pixels mm$^{-1}$
rotation method scans
30357 measured reflections
7337 independent reflections
22778 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.035
$\theta_{max}$ = 25.5°, $\theta_{min}$ = 2.6°
$h$ = −13→13
$k$ = −34→38
$l$ = −13→13

Refinement

Refinement on $F^2$
Least-squares matrix: full
$R(F^2 > 2\sigma(F^2))$ = 0.048
$wR(F^2) = 0.118$
$S$ = 1.06
30357 reflections
1000 parameters
9 restraints
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_c^2) + (0.0264P)^2 + 2.6942P]$
where $P = (F_c^2 + 2F_s^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta$ρ$_{max}$ = 0.35 e Å$^{-3}$
$\Delta$ρ$_{min}$ = −0.47 e Å$^{-3}$
Absolute structure: Flack $x$ determined using 3722 quotients [(I$^+$)+(I$^-$)]/[I$^+$]+(I$^-$)] (Parsons et al., 2013)
Absolute structure parameter: −0.13 (5)
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    | Uiso*/Ueq |
|----|------|------|------|-----------|
| N1 | 0.9085 (4) | 0.49651 (17) | 0.3802 (5) | 0.0304 (12) |
| N2 | 1.0161 (4) | 0.48419 (18) | 0.4341 (5) | 0.0348 (13) |
| N3 | 0.7756 (4) | 0.32258 (16) | 0.5118 (4) | 0.0266 (11) |
| N4 | 0.8876 (4) | 0.33661 (17) | 0.4826 (5) | 0.0296 (12) |
| N5 | 0.9558 (5) | 0.42548 (19) | 0.9122 (5) | 0.0392 (14) |
| N6 | 1.0494 (5) | 0.4218 (2)   | 0.8367 (6) | 0.0471 (16) |
| C1 | 0.7875 (5) | 0.46663 (19) | 0.5401 (5) | 0.0266 (13) |
| C2 | 0.7354 (5) | 0.42832 (19) | 0.4989 (5) | 0.0265 (13) |
| C3 | 0.7276 (5) | 0.3944 (2)   | 0.5786 (5) | 0.0268 (13) |
| C4 | 0.7670 (5) | 0.3987 (2)   | 0.7000 (5) | 0.0275 (13) |
| C5 | 0.8109 (5) | 0.4377 (2)   | 0.7412 (5) | 0.0291 (14) |
| C6 | 0.8262 (5) | 0.4718 (2)   | 0.6611 (6) | 0.0290 (14) |
| C7 | 0.8034 (5) | 0.5025 (2)   | 0.4525 (6) | 0.0298 (14) |
| H7E| 0.7304 | 0.5047 | 0.3985 | 0.036* |
| H7F| 0.8122 | 0.5294 | 0.4975 | 0.036* |
| C8 | 1.0981 (6) | 0.4895 (2) | 0.3517 (6) | 0.0357 (16) |
| H8 | 1.1813 | 0.4833 | 0.3646 | 0.043* |
| C9 | 1.0454 (6) | 0.5055 (2) | 0.2423 (6) | 0.0321 (15) |
| C10| 1.0879 (6) | 0.5153 (2) | 0.1284 (6) | 0.0385 (16) |
| C11| 1.0028 (7) | 0.5307 (2) | 0.0453 (6) | 0.0434 (18) |
| H11| 1.0279 | 0.5381 | −0.0321 | 0.052* |
| C12| 0.8803 (7) | 0.5360 (2) | 0.0698 (6) | 0.0402 (17) |
| H12| 0.8261 | 0.5468 | 0.0090 | 0.048* |
| C13| 0.8378 (6) | 0.5256 (2) | 0.1802 (6) | 0.0351 (15) |
| H13| 0.7555 | 0.5289 | 0.1972 | 0.042* |
| C14| 0.9221 (6) | 0.5102 (2) | 0.2652 (5) | 0.0300 (14) |
| C15| 0.6879 (5) | 0.4241 (2) | 0.3692 (5) | 0.0339 (15) |
| H15A| 0.7032 | 0.3951 | 0.3405 | 0.041* |
| H15B| 0.7316 | 0.4441 | 0.3185 | 0.041* |
| C16| 0.5531 (6) | 0.4335 (3) | 0.3563 (6) | 0.0441 (18) |
| H16A| 0.5265 | 0.4323 | 0.2713 | 0.066* |
| H16B| 0.5373 | 0.4617 | 0.3882 | 0.066* |
| H16C| 0.5090 | 0.4123 | 0.4010 | 0.066* |
| C17| 0.6785 (5) | 0.35214 (19) | 0.5355 (6) | 0.0297 (14) |
| H17A| 0.6274 | 0.3400 | 0.5971 | 0.036* |
| H17B| 0.6276 | 0.3563 | 0.4612 | 0.036* |
| C18| 0.9527 (5) | 0.3017 (2) | 0.4662 (5) | 0.0315 (14) |
| H18| 1.0343 | 0.3017 | 0.4446 | 0.038* |
| Atom | X       | Y       | Z       | U ^{1}   | U ^{2}   | U ^{3}   | U ^{4} | U ^{5} | U ^{6} | U ^{7} | U ^{8} |
|------|---------|---------|---------|----------|----------|----------|--------|--------|--------|--------|--------|
| C19  | 0.8845(5) | 0.2646(2) | 0.4851(5) | 0.0273(13) |        |          |        |        |        |        |        |
| C20  | 0.9092(5) | 0.2207(2) | 0.4841(5) | 0.0282(14) |        |          |        |        |        |        |        |
| C21  | 0.8169(5) | 0.1942(2) | 0.5128(6) | 0.0341(15) |        |          |        |        |        |        |        |
| H21  | 0.8305    | 0.1645   | 0.5138   | 0.041*    |        |          |        |        |        |        |        |
| C22  | 0.7016(6) | 0.2098(2) | 0.5411(6) | 0.0342(15) |        |          |        |        |        |        |        |
| H22  | 0.6405    | 0.1901   | 0.5596   | 0.041*    |        |          |        |        |        |        |        |
| C23  | 0.6761(5) | 0.2522(2) | 0.5422(6) | 0.0314(14) |        |          |        |        |        |        |        |
| H23  | 0.5991    | 0.2626   | 0.5609   | 0.038*    |        |          |        |        |        |        |        |
| C24  | 0.7701(5) | 0.2794(2) | 0.5144(5) | 0.0263(13) |        |          |        |        |        |        |        |
| C25  | 0.7677(6) | 0.3604(2) | 0.7833(6) | 0.0351(15) |        |          |        |        |        |        |        |
| H25A | 0.8347    | 0.3638   | 0.8442   | 0.042*    |        |          |        |        |        |        |        |
| H25B | 0.7846    | 0.3349   | 0.7356   | 0.042*    |        |          |        |        |        |        |        |
| C26  | 0.6512(6) | 0.3529(3) | 0.8488(6) | 0.0439(18)|        |          |        |        |        |        |        |
| H26A | 0.5832    | 0.3508   | 0.7899   | 0.066*    |        |          |        |        |        |        |        |
| H26B | 0.6380    | 0.3765   | 0.9035   | 0.066*    |        |          |        |        |        |        |        |
| C27  | 0.8407(6) | 0.4431(2) | 0.8731(6) | 0.0383(16)|        |          |        |        |        |        |        |
| H27A | 0.8403    | 0.4737   | 0.8926   | 0.046*    |        |          |        |        |        |        |        |
| H27B | 0.7770    | 0.4294   | 0.9186   | 0.046*    |        |          |        |        |        |        |        |
| C28  | 1.1413(6) | 0.4071(3) | 0.9048(8) | 0.052(2)  |        |          |        |        |        |        |        |
| H28  | 1.2185    | 0.4010   | 0.8765   | 0.062*    |        |          |        |        |        |        |        |
| C29  | 1.1087(7) | 0.4017(2) | 1.0265(7) | 0.0446(18)|        |          |        |        |        |        |        |
| C30  | 1.1714(7) | 0.3876(2) | 1.1362(8) | 0.051(2)  |        |          |        |        |        |        |        |
| C31  | 1.1012(7) | 0.3872(3) | 1.2350(7) | 0.0505(19)|        |          |        |        |        |        |        |
| H31  | 1.1390    | 0.3792   | 1.3098   | 0.061*    |        |          |        |        |        |        |        |
| C32  | 0.9806(8) | 0.3976(3) | 1.2336(7) | 0.056(2)  |        |          |        |        |        |        |        |
| H32  | 0.9379    | 0.3948   | 1.3049   | 0.067*    |        |          |        |        |        |        |        |
| C33  | 0.9214(7) | 0.4118(2) | 1.1306(6) | 0.0485(19)|        |          |        |        |        |        |        |
| H33  | 0.8392    | 0.4200   | 1.1290   | 0.058*    |        |          |        |        |        |        |        |
| C34  | 0.9888(7) | 0.4136(2) | 1.0285(6) | 0.0396(17)|        |          |        |        |        |        |        |
| C35  | 0.8893(6) | 0.5120(2) | 0.7032(6) | 0.0344(15)|        |          |        |        |        |        |        |
| H35A | 0.9403    | 0.5223   | 0.6389   | 0.041*    |        |          |        |        |        |        |        |
| H35B | 0.9429    | 0.5054   | 0.7742   | 0.041*    |        |          |        |        |        |        |        |
| C36  | 0.8030(6) | 0.5476(2) | 0.7363(6) | 0.0415(17)|        |          |        |        |        |        |        |
| H36A | 0.8495    | 0.5726   | 0.7624   | 0.062*    |        |          |        |        |        |        |        |
| H36B | 0.7536    | 0.5380   | 0.8015   | 0.062*    |        |          |        |        |        |        |        |
| H36C | 0.7508    | 0.5548   | 0.6661   | 0.062*    |        |          |        |        |        |        |        |
| C37  | 1.2173(6) | 0.5090(3) | 0.1021(7) | 0.049(2)  |        |          |        |        |        |        |        |
| H37A | 1.2309    | 0.5185   | 0.0202   | 0.074*    |        |          |        |        |        |        |        |
| H37B | 1.2376    | 0.4789   | 0.1095   | 0.074*    |        |          |        |        |        |        |        |
| H37C | 1.2683    | 0.5253   | 0.1592   | 0.074*    |        |          |        |        |        |        |        |
| C38  | 1.0334(6) | 0.2056(2) | 0.4556(6) | 0.0400(17)|        |          |        |        |        |        |        |
| H38A | 1.0337    | 0.1746   | 0.4501   | 0.060*    |        |          |        |        |        |        |        |
| H38B | 1.0915    | 0.2147   | 0.5192   | 0.060*    |        |          |        |        |        |        |        |
| H38C | 1.0557    | 0.2177   | 0.3788   | 0.060*    |        |          |        |        |        |        |        |
| C39  | 1.2989(7) | 0.3748(3) | 1.1338(9) | 0.069(3)  |        |          |        |        |        |        |        |
| H39A | 1.3078    | 0.3531   | 1.0721   | 0.104*    |        |          |        |        |        |        |        |
| H39B | 1.3255    | 0.3634   | 1.2123   | 0.104*    |        |          |        |        |        |        |        |
|   |   |   |   |   |
|---|---|---|---|---|
| H39C | 1.3481 | 0.3995 | 1.1153 | 0.104* |
| P1  | 0.32584 (14) | 0.32786 (6) | 0.55803 (18) | 0.0391 (4) |
| F1  | 0.4117 (4) | 0.36199 (16) | 0.6156 (5) | 0.0707 (15) |
| F2  | 0.2398 (4) | 0.2950 (3) | 0.4939 (9) | 0.160 (4) |
| F3  | 0.2545 (5) | 0.3639 (2) | 0.4858 (4) | 0.102 (2) |
| F4  | 0.3958 (5) | 0.2928 (2) | 0.6297 (6) | 0.105 (2) |
| F5  | 0.2338 (4) | 0.33518 (17) | 0.6590 (5) | 0.0798 (17) |
| F6  | 0.4149 (4) | 0.32195 (18) | 0.4524 (4) | 0.0685 (15) |
| N7  | 0.0426 (5) | 0.4071 (2) | 0.5778 (6) | 0.0366 (13) |
| H7A | 0.039 (8) | 0.4325 (17) | 0.539 (8) | 0.10 (4)* |
| H7B | −0.018 (6) | 0.389 (2) | 0.554 (8) | 0.08 (3)* |
| H7C | 0.041 (7) | 0.413 (3) | 0.658 (3) | 0.08 (3)* |
| H7D | 0.116 (4) | 0.396 (2) | 0.562 (7) | 0.06 (2)* |
| N1A | 0.6736 (4) | 0.74922 (16) | 0.8989 (4) | 0.0280 (11) |
| N2A | 0.6283 (4) | 0.73648 (18) | 1.0056 (5) | 0.0324 (12) |
| N3A | 0.4984 (4) | 0.57729 (16) | 0.7628 (4) | 0.0271 (11) |
| N4A | 0.5334 (4) | 0.59050 (16) | 0.8767 (4) | 0.0299 (12) |
| N5A | 0.1345 (4) | 0.68517 (17) | 0.9421 (4) | 0.0284 (12) |
| N6A | 0.2162 (4) | 0.68319 (18) | 1.0390 (5) | 0.0334 (13) |
| C1A | 0.4987 (5) | 0.72111 (19) | 0.7775 (5) | 0.0251 (13) |
| C2A | 0.5286 (5) | 0.68253 (19) | 0.7258 (5) | 0.0255 (13) |
| C3A | 0.4406 (5) | 0.65035 (19) | 0.7139 (5) | 0.0250 (13) |
| C4A | 0.3227 (5) | 0.6572 (2) | 0.7494 (5) | 0.0269 (13) |
| C5A | 0.2945 (5) | 0.6967 (2) | 0.7980 (5) | 0.0264 (13) |
| C6A | 0.3817 (5) | 0.72862 (19) | 0.8166 (5) | 0.0263 (13) |
| C7A | 0.5933 (5) | 0.7559 (2) | 0.7927 (5) | 0.0294 (14) |
| H7AE| 0.6417 | 0.7568 | 0.7205 | 0.035* |
| H7AF| 0.5525 | 0.7836 | 0.7996 | 0.035* |
| C8A | 0.7164 (5) | 0.7422 (2) | 1.0901 (6) | 0.0326 (15) |
| H8A | 0.7096 | 0.7357 | 1.1727 | 0.039* |
| C9A | 0.8212 (5) | 0.7593 (2) | 1.0407 (6) | 0.0296 (14) |
| C10A| 0.9367 (5) | 0.7707 (2) | 1.0880 (6) | 0.0331 (15) |
| C11A| 1.0136 (6) | 0.7872 (2) | 1.0064 (6) | 0.0372 (16) |
| H11A| 1.0926 | 0.7950 | 1.0340 | 0.045* |
| C12A| 0.9802 (5) | 0.7930 (2) | 0.8837 (6) | 0.0364 (16) |
| H12A| 1.0360 | 0.8054 | 0.8323 | 0.044* |
| C13A| 0.8678 (5) | 0.7810 (2) | 0.8369 (6) | 0.0333 (15) |
| H13A| 0.8457 | 0.7843 | 0.7541 | 0.040* |
| C14A| 0.7891 (5) | 0.7640 (2) | 0.9170 (5) | 0.0269 (13) |
| C15A| 0.6532 (5) | 0.6762 (2) | 0.6767 (6) | 0.0338 (15) |
| H15C| 0.6806 | 0.6468 | 0.6932 | 0.041* |
| H15D| 0.7111 | 0.6958 | 0.7178 | 0.041* |
| C16A| 0.6503 (6) | 0.6844 (3) | 0.5414 (6) | 0.0411 (17) |
| H16D| 0.7284 | 0.6769 | 0.5102 | 0.062* |
| H16E| 0.6335 | 0.7144 | 0.5258 | 0.062* |
| H16F| 0.5872 | 0.6670 | 0.5016 | 0.062* |
| C17A| 0.4759 (6) | 0.6079 (2) | 0.6649 (5) | 0.0311 (14) |
| H17C| 0.4106 | 0.5972 | 0.6094 | 0.037* |
| Atom | x     | y     | z     | U(eq)  |
|------|-------|-------|-------|--------|
| H17D | 0.5494| 0.6111| 0.6191| 0.037* |
| C18A | 0.5432 (5) | 0.5556 (2) | 0.9440 (6) | 0.0329 (15) |
| H18A | 0.5667 | 0.5552 | 1.0270 | 0.040* |
| C19A | 0.5136 (5) | 0.5190 (2) | 0.8743 (6) | 0.0298 (14) |
| C20A | 0.5069 (6) | 0.4752 (2) | 0.8989 (6) | 0.0347 (15) |
| C21A | 0.4720 (6) | 0.4496 (2) | 0.8037 (6) | 0.0426 (17) |
| H21A | 0.4657 | 0.4199 | 0.8170 | 0.051* |
| C22A | 0.4449 (6) | 0.4654 (2) | 0.6864 (6) | 0.0407 (17) |
| H22A | 0.4213 | 0.4462 | 0.6241 | 0.049* |
| C23A | 0.4521 (6) | 0.5079 (2) | 0.6607 (6) | 0.0365 (16) |
| H23A | 0.4353 | 0.5187 | 0.5821 | 0.044* |
| C24A | 0.4857 (5) | 0.5345 (2) | 0.7572 (5) | 0.0275 (13) |
| C25A | 0.2276 (6) | 0.6230 (2) | 0.7317 (6) | 0.0366 (16) |
| H25C | 0.2454 | 0.6064 | 0.6594 | 0.044* |
| C26A | 0.1485 | 0.6369 | 0.7160 | 0.044* |
| C26D | 0.2175 (6) | 0.5923 (2) | 0.8377 (6) | 0.0375 (16) |
| C26E | 0.1556 | 0.5711 | 0.8177 | 0.056* |
| C26F | 0.1956 | 0.6082 | 0.9090 | 0.056* |
| C27A | 0.2950 | 0.5782 | 0.8539 | 0.056* |
| C27C | 0.1663 (5) | 0.7057 (2) | 0.8315 (6) | 0.0342 (15) |
| C27D | 0.1557 | 0.7366 | 0.8401 | 0.041* |
| C27E | 0.1103 | 0.6960 | 0.7655 | 0.041* |
| C28A | 0.1567 (5) | 0.6664 (2) | 1.1291 (6) | 0.0334 (15) |
| C28C | 0.1915 | 0.6607 | 1.2069 | 0.040* |
| C29A | 0.0342 (5) | 0.6583 (2) | 1.0929 (5) | 0.0270 (13) |
| C29C | 0.3068 (5) | 0.6416 (2) | 1.1511 (6) | 0.0313 (14) |
| C31A | 0.1721 (6) | 0.6383 (2) | 1.0830 (6) | 0.0344 (15) |
| C31B | 0.2416 | 0.6279 | 1.1195 | 0.041* |
| C32A | 0.1808 (5) | 0.6499 (2) | 0.9607 (6) | 0.0350 (15) |
| C32B | 0.2555 | 0.6463 | 0.9169 | 0.042* |
| C33A | 0.0843 (5) | 0.6662 (2) | 0.9025 (6) | 0.0314 (14) |
| C33B | 0.0905 | 0.6740 | 0.8202 | 0.038* |
| C34A | 0.2415 (5) | 0.67062 (19) | 0.9726 (5) | 0.0265 (14) |
| C35A | 0.3533 (6) | 0.7695 (2) | 0.8800 (6) | 0.0323 (14) |
| C35C | 0.4262 | 0.7792 | 0.9266 | 0.039* |
| C35D | 0.2900 | 0.7640 | 0.9375 | 0.039* |
| C36A | 0.3105 (6) | 0.8051 (2) | 0.7941 (6) | 0.0374 (16) |
| C36C | 0.3742 | 0.8118 | 0.7395 | 0.056* |
| C36D | 0.2917 | 0.8304 | 0.8406 | 0.056* |
| C36E | 0.2383 | 0.7959 | 0.7475 | 0.056* |
| C37A | 0.9719 (6) | 0.7650 (2) | 1.2184 (6) | 0.0438 (18) |
| C37D | 0.9614 | 0.7353 | 1.2407 | 0.066* |
| C37E | 0.9210 | 0.7829 | 1.2667 | 0.066* |
| C37F | 1.0564 | 0.7731 | 1.2329 | 0.066* |
| C38A | 0.5366 (7) | 0.4596 (2) | 1.0237 (6) | 0.0450 (18) |
| C38D | 0.5299 | 0.4287 | 1.0256 | 0.067* |
| C38E | 0.4804 | 0.4720 | 1.0789 | 0.067* |
| C38F | 0.6190 | 0.4680 | 1.0482 | 0.067* |
### Atomic displacement parameters (Å²)

|     | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|-----|----------|----------|----------|----------|----------|----------|
| N1  | 0.034    | 0.032    | 0.025    | 0.002    | 0.003    | 0.006    |
| N2  | 0.032    | 0.039    | 0.033    | 0.005    | 0.001    | 0.002    |
| N3  | 0.022    | 0.025    | 0.033    | 0.002    | 0.0044   | −0.002   |
| N4  | 0.024    | 0.033    | 0.032    | 0.001    | 0.004    | 0.000    |
| N5  | 0.049    | 0.043    | 0.025    | −0.005   | −0.004   | 0.003    |
| N6  | 0.038    | 0.053    | 0.049    | −0.004   | −0.011   | 0.011    |
| C1  | 0.028    | 0.025    | 0.027    | 0.003    | 0.003    | 0.004    |
| C2  | 0.029    | 0.024    | 0.026    | 0.005    | 0.003    | 0.004    |
| C3  | 0.025    | 0.030    | 0.027    | 0.004    | 0.004    | 0.001    |
| C4  | 0.032    | 0.028    | 0.024    | 0.004    | 0.004    | 0.003    |
| C5  | 0.035    | 0.027    | 0.024    | 0.001    | 0.001    | 0.003    |
| C6  | 0.032    | 0.025    | 0.030    | 0.003    | 0.003    | 0.000    |
| C7  | 0.031    | 0.031    | 0.029    | 0.002    | 0.009    | 0.003    |
| C8  | 0.035    | 0.038    | 0.034    | −0.003   | 0.006    | −0.001   |
| C9  | 0.040    | 0.029    | 0.028    | −0.007   | 0.009    | 0.000    |
| C10 | 0.046    | 0.036    | 0.035    | −0.016   | 0.013    | −0.004   |
| C11 | 0.066    | 0.039    | 0.026    | −0.017   | 0.007    | 0.001    |
| C12 | 0.063    | 0.030    | 0.028    | −0.006   | 0.000    | 0.002    |
| C13 | 0.046    | 0.028    | 0.031    | −0.006   | −0.002   | 0.003    |
| C14 | 0.042    | 0.025    | 0.023    | −0.002   | 0.005    | 0.001    |
| C15 | 0.044    | 0.035    | 0.023    | −0.001   | −0.001   | 0.003    |
| C16 | 0.048    | 0.052    | 0.031    | 0.001    | −0.010   | 0.006    |
| C17 | 0.027    | 0.027    | 0.035    | 0.004    | 0.003    | 0.000    |
| C18 | 0.031    | 0.033    | 0.031    | 0.002    | 0.003    | 0.001    |
| C19 | 0.025    | 0.030    | 0.027    | 0.000    | 0.001    | −0.002   |
| C20 | 0.028    | 0.033    | 0.024    | 0.006    | −0.003   | −0.003   |
| C21 | 0.036    | 0.030    | 0.035    | 0.001    | −0.004   | −0.003   |
| C22 | 0.035    | 0.028    | 0.039    | −0.005   | −0.001   | 0.002    |
| Atom | U11  | U22  | U33  | U12 | U13 | U23 |
|------|------|------|------|-----|-----|-----|
| C23  | 0.026 (3) | 0.034 (4) | 0.035 (4) | -0.004 (3) | 0.002 (2) | 0.003 (3) |
| C24  | 0.024 (3) | 0.027 (3) | 0.027 (3) | -0.002 (2) | 0.000 (2) | 0.000 (3) |
| C25  | 0.041 (4) | 0.031 (4) | 0.033 (4) | 0.004 (3) | 0.000 (3) | 0.003 (3) |
| C26  | 0.045 (4) | 0.049 (5) | 0.039 (4) | 0.001 (3) | 0.009 (3) | 0.013 (3) |
| C27  | 0.051 (4) | 0.042 (4) | 0.022 (3) | 0.004 (3) | 0.000 (3) | 0.004 (3) |
| C28  | 0.033 (4) | 0.056 (5) | 0.065 (6) | -0.005 (3) | -0.012 (3) | 0.012 (4) |
| C29  | 0.058 (5) | 0.034 (4) | 0.041 (5) | -0.013 (3) | -0.013 (3) | 0.006 (3) |
| C30  | 0.062 (5) | 0.025 (4) | 0.064 (6) | -0.009 (3) | -0.021 (4) | 0.001 (4) |
| C31  | 0.069 (5) | 0.044 (5) | 0.037 (5) | -0.008 (4) | -0.010 (4) | -0.001 (4) |
| C32  | 0.085 (6) | 0.040 (5) | 0.042 (5) | -0.004 (4) | -0.006 (4) | 0.008 (4) |
| C33  | 0.072 (5) | 0.044 (5) | 0.044 (4) | 0.009 (3) | -0.001 (3) | -0.003 (3) |
| C34  | 0.069 (5) | 0.054 (6) | 0.093 (7) | -0.017 (4) | -0.023 (5) | 0.024 (5) |
| P1   | 0.0251 (9) | 0.0406 (11) | 0.0514 (12) | 0.0037 (8) | -0.0008 (7) | -0.0073 (9) |
| F1   | 0.042 (2) | 0.069 (3) | 0.101 (4) | -0.007 (2) | 0.002 (2) | -0.046 (3) |
| F2   | 0.028 (3) | 0.140 (6) | 0.314 (11) | -0.021 (3) | 0.010 (4) | -0.149 (7) |
| F3   | 0.107 (4) | 0.153 (6) | 0.046 (3) | 0.092 (4) | -0.006 (3) | 0.009 (3) |
| F4   | 0.106 (4) | 0.079 (4) | 0.134 (5) | 0.058 (4) | 0.043 (4) | 0.052 (4) |
| F5   | 0.065 (3) | 0.074 (4) | 0.105 (4) | 0.016 (3) | 0.055 (3) | 0.016 (3) |
| F6   | 0.050 (3) | 0.103 (4) | 0.053 (3) | 0.019 (3) | 0.012 (2) | -0.029 (3) |
| N7   | 0.031 (3) | 0.033 (4) | 0.045 (4) | 0.005 (3) | -0.001 (3) | 0.002 (3) |
| N3A  | 0.032 (3) | 0.039 (3) | 0.026 (3) | -0.004 (2) | 0.000 (2) | 0.002 (2) |
| N4A  | 0.033 (3) | 0.033 (4) | 0.023 (3) | 0.001 (2) | 0.000 (2) | 0.002 (2) |
| N5A  | 0.030 (3) | 0.025 (3) | 0.023 (3) | -0.003 (2) | 0.000 (2) | 0.002 (2) |
| N6A  | 0.032 (3) | 0.029 (3) | 0.020 (3) | -0.001 (2) | 0.001 (2) | 0.002 (2) |
| C1A  | 0.026 (3) | 0.026 (3) | 0.026 (3) | -0.002 (2) | 0.000 (2) | 0.002 (2) |
| C2A  | 0.025 (3) | 0.027 (3) | 0.027 (3) | -0.001 (2) | 0.001 (2) | 0.000 (3) |
| C3A  | 0.031 (3) | 0.021 (3) | 0.023 (3) | -0.002 (2) | 0.000 (2) | 0.001 (3) |
| C4A  | 0.028 (3) | 0.029 (4) | 0.023 (3) | -0.003 (2) | -0.001 (2) | 0.004 (3) |
| C5A  | 0.023 (3) | 0.030 (3) | 0.027 (3) | -0.001 (2) | 0.000 (2) | 0.003 (3) |
| C6A  | 0.026 (3) | 0.026 (3) | 0.026 (3) | 0.003 (2) | -0.002 (2) | 0.001 (3) |
| C7A  | 0.031 (3) | 0.030 (4) | 0.027 (3) | -0.005 (3) | -0.005 (2) | 0.004 (3) |
| C8A  | 0.032 (3) | 0.040 (4) | 0.026 (3) | -0.002 (3) | -0.002 (3) | -0.002 (3) |
| C9A  | 0.023 (3) | 0.030 (4) | 0.036 (4) | 0.000 (2) | 0.000 (2) | -0.005 (3) |
| C10A | 0.029 (3) | 0.028 (4) | 0.041 (4) | 0.003 (3) | -0.007 (3) | -0.008 (3) |
| C11A | 0.028 (3) | 0.033 (4) | 0.050 (4) | 0.000 (3) | 0.000 (3) | -0.009 (3) |
| C12A | 0.028 (3) | 0.032 (4) | 0.050 (4) | -0.001 (3) | 0.006 (3) | -0.002 (3) |
| C13A | 0.027 (3) | 0.030 (4) | 0.043 (4) | 0.000 (3) | 0.003 (3) | -0.001 (3) |
| C14A | 0.024 (3) | 0.026 (3) | 0.030 (3) | -0.002 (2) | -0.001 (2) | 0.000 (3) |
| C15A | 0.026 (3) | 0.042 (4) | 0.034 (4) | 0.001 (3) | 0.004 (2) | -0.007 (3) |
| C16A | 0.036 (4) | 0.057 (5) | 0.032 (4) | -0.008 (3) | 0.011 (3) | 0.001 (3) |
| C17A | 0.047 (4) | 0.025 (3) | 0.021 (3) | 0.005 (3) | 0.001 (3) | 0.004 (3) |

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Geometric parameters (Å, º)

|   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|
|N1—C14 | 1.369 (8) | N1A—C14A | 1.372 (7) |
|N1—N2 | 1.370 (7) | N1A—N2A | 1.376 (7) |
|N1—C7 | 1.465 (7) | N1A—C7A | 1.465 (7) |
|N2—C8 | 1.336 (8) | N2A—C8A | 1.339 (8) |
|N3—C24 | 1.367 (8) | N3A—C24A | 1.362 (8) |
|N3—N4 | 1.377 (7) | N3A—N4A | 1.377 (7) |
|N3—C17 | 1.461 (7) | N3A—C17A | 1.471 (8) |
|N4—C18 | 1.337 (8) | N4A—C18A | 1.335 (8) |
|N5—N6 | 1.375 (8) | N5A—C34A | 1.369 (7) |
|N5—C34 | 1.383 (8) | N5A—N6A | 1.380 (7) |
|N5—C27 | 1.445 (8) | N5A—C27A | 1.452 (8) |
|N6—C28 | 1.327 (9) | N6A—C28A | 1.339 (8) |
|C1—C6 | 1.407 (8) | C1A—C2A | 1.395 (8) |
|C1—C2 | 1.410 (9) | C1A—C6A | 1.413 (8) |
|C1—C7 | 1.513 (8) | C1A—C7A | 1.525 (8) |
| Bond          | Length (Å) | Bond          | Length (Å) | Bond          | Length (Å) |
|--------------|------------|--------------|------------|--------------|------------|
| C2—C3        | 1.398 (8)  | C2A—C3A      | 1.413 (8)  |              |            |
| C2—C15       | 1.521 (8)  | C2A—C15A     | 1.528 (8)  |              |            |
| C3—C4        | 1.409 (8)  | C3A—C4A      | 1.405 (8)  |              |            |
| C3—C17       | 1.512 (9)  | C3A—C17A     | 1.507 (9)  |              |            |
| C4—C5        | 1.396 (9)  | C4A—C5A      | 1.403 (9)  |              |            |
| C4—C25       | 1.524 (9)  | C4A—C25A     | 1.518 (8)  |              |            |
| C5—C6        | 1.414 (9)  | C5A—C6A      | 1.407 (8)  |              |            |
| C5—C27       | 1.503 (9)  | C5A—C27A     | 1.518 (8)  |              |            |
| C6—C35       | 1.516 (9)  | C6A—C35A     | 1.514 (8)  |              |            |
| C7—H7E       | 0.9900     | C7A—H7AE     | 0.9900     |              |            |
| C7—H7F       | 0.9900     | C7A—H7AF     | 0.9900     |              |            |
| C8—C9        | 1.422 (9)  | C8A—C9A      | 1.420 (9)  |              |            |
| C8—H8        | 0.9500     | C8A—H8A      | 0.9500     |              |            |
| C9—C10       | 1.412 (9)  | C9A—C10A     | 1.411 (8)  |              |            |
| C9—C14       | 1.415 (9)  | C9A—C14A     | 1.417 (9)  |              |            |
| C10—C11      | 1.380 (10) | C10A—C11A    | 1.382 (10) |              |            |
| C10—C37      | 1.497 (10) | C10A—C37A    | 1.499 (9)  |              |            |
| C11—C12      | 1.412 (10) | C11A—C12A    | 1.413 (9)  |              |            |
| C11—H11      | 0.9500     | C11A—H11A    | 0.9500     |              |            |
| C12—C13      | 1.379 (9)  | C12A—C13A    | 1.384 (8)  |              |            |
| C12—H12      | 0.9500     | C12A—H12A    | 0.9500     |              |            |
| C13—C14      | 1.390 (9)  | C13A—C14A    | 1.390 (9)  |              |            |
| C13—C15      | 0.9500     | C13A—C15A    | 0.9500     |              |            |
| C15—C16      | 1.529 (9)  | C15A—C16A    | 1.530 (9)  |              |            |
| C15—H15A     | 0.9900     | C15A—H15C    | 0.9900     |              |            |
| C15—H15B     | 0.9900     | C15A—H15D    | 0.9900     |              |            |
| C16—H16A     | 0.9800     | C16A—H16D    | 0.9800     |              |            |
| C16—H16B     | 0.9800     | C16A—H16E    | 0.9800     |              |            |
| C16—H16C     | 0.9800     | C16A—H16F    | 0.9800     |              |            |
| C17—H17A     | 0.9900     | C17A—H17C    | 0.9900     |              |            |
| C17—H17B     | 0.9900     | C17A—H17D    | 0.9900     |              |            |
| C18—C19      | 1.416 (9)  | C18A—C19A    | 1.423 (9)  |              |            |
| C18—H18      | 0.9500     | C18A—H18A    | 0.9500     |              |            |
| C19—C24      | 1.409 (8)  | C19A—C20A    | 1.413 (9)  |              |            |
| C19—C20      | 1.415 (9)  | C19A—C24A    | 1.415 (9)  |              |            |
| C20—C21      | 1.373 (9)  | C20A—C21A    | 1.376 (10) |              |            |
| C20—C38      | 1.511 (8)  | C20A—C38A    | 1.499 (9)  |              |            |
| C21—C22      | 1.423 (9)  | C21A—C22A    | 1.420 (10) |              |            |
| C21—H21      | 0.9500     | C21A—H21A    | 0.9500     |              |            |
| C22—C23      | 1.371 (9)  | C22A—C23A    | 1.376 (10) |              |            |
| C22—H22      | 0.9500     | C22A—H22A    | 0.9500     |              |            |
| C23—C24      | 1.398 (8)  | C23A—C24A    | 1.401 (9)  |              |            |
| C23—H23      | 0.9500     | C23A—H23A    | 0.9500     |              |            |
| C25—C26      | 1.536 (9)  | C25A—C26A    | 1.537 (9)  |              |            |
| C25—H25A     | 0.9900     | C25A—H25C    | 0.9900     |              |            |
| C25—H25B     | 0.9900     | C25A—H25D    | 0.9900     |              |            |
| C26—H26A     | 0.9800     | C26A—H26D    | 0.9800     |              |            |
| C26—H26B     | 0.9800     | C26A—H26E    | 0.9800     |              |            |
### Supporting Information

| Bond                  | Distance (Å) | Bond                  | Distance (Å) | Bond                  | Distance (Å) |
|-----------------------|--------------|-----------------------|--------------|-----------------------|--------------|
| C26—H26C              | 0.9800       | C26A—H26F             | 0.9800       |                       |              |
| C27—H27A              | 0.9900       | C27A—H27C             | 0.9900       |                       |              |
| C27—H27B              | 0.9900       | C27A—H27D             | 0.9900       |                       |              |
| C28—C29               | 1.432 (11)   | C28A—C29A             | 1.426 (8)    |                       |              |
| C28—H28               | 0.9500       | C28A—H28A             | 0.9500       |                       |              |
| C29—C34               | 1.387 (10)   | C29A—C34A             | 1.397 (8)    |                       |              |
| C29—C30               | 1.449 (10)   | C29A—C30A             | 1.417 (8)    |                       |              |
| C30—C31               | 1.381 (12)   | C30A—C31A             | 1.378 (9)    |                       |              |
| C30—C39               | 1.477 (11)   | C30A—C39A             | 1.496 (9)    |                       |              |
| C31—C32               | 1.381 (11)   | C31A—C32A             | 1.412 (9)    |                       |              |
| C31—H31               | 0.9500       | C31A—H31A             | 0.9500       |                       |              |
| C32—C33               | 1.372 (10)   | C32A—C33A             | 1.381 (9)    |                       |              |
| C32—H32               | 0.9500       | C32A—H32A             | 0.9500       |                       |              |
| C33—C34               | 1.395 (11)   | C33A—C34A             | 1.413 (8)    |                       |              |
| C33—H33               | 0.9500       | C33A—H33A             | 0.9500       |                       |              |
| C35—C36               | 1.534 (9)    | C35A—C36A             | 1.538 (9)    |                       |              |
| C35—H35A              | 0.9900       | C35A—H35C             | 0.9900       |                       |              |
| C35—H35B              | 0.9900       | C35A—H35D             | 0.9900       |                       |              |
| C36—H36A              | 0.9800       | C36A—H36D             | 0.9800       |                       |              |
| C36—H36B              | 0.9800       | C36A—H36E             | 0.9800       |                       |              |
| C36—H36C              | 0.9800       | C36A—H36F             | 0.9800       |                       |              |
| C37—H37A              | 0.9800       | C37A—H37D             | 0.9800       |                       |              |
| C37—H37B              | 0.9800       | C37A—H37E             | 0.9800       |                       |              |
| C37—H37C              | 0.9800       | C37A—H37F             | 0.9800       |                       |              |
| C38—H38A              | 0.9800       | C38A—H38D             | 0.9800       |                       |              |
| C38—H38B              | 0.9800       | C38A—H38E             | 0.9800       |                       |              |
| C38—H38C              | 0.9800       | C38A—H38F             | 0.9800       |                       |              |
| C39—H39A              | 0.9800       | C39A—H39D             | 0.9800       |                       |              |
| C39—H39B              | 0.9800       | C39A—H39E             | 0.9800       |                       |              |
| C39—H39C              | 0.9800       | C39A—H39F             | 0.9800       |                       |              |
| P1—F4                 | 1.552 (5)    | P1A—F1A               | 1.593 (4)    |                       |              |
| P1—F1                 | 1.558 (5)    | P1A—F2A               | 1.599 (4)    |                       |              |
| P1—F2                 | 1.561 (5)    | P1A—F3A               | 1.598 (5)    |                       |              |
| P1—F5                 | 1.575 (5)    | P1A—F4A               | 1.587 (4)    |                       |              |
| P1—F3                 | 1.585 (5)    | P1A—F5A               | 1.579 (4)    |                       |              |
| P1—F6                 | 1.587 (5)    | P1A—F6A               | 1.590 (5)    |                       |              |
| N7—H7A                | 0.91 (2)     | N7A—H7AA              | 0.91 (2)     |                       |              |
| N7—H7B                | 0.91 (2)     | N7A—H7AB              | 0.91 (2)     |                       |              |
| N7—H7C                | 0.91 (2)     | N7A—H7AC              | 0.92 (2)     |                       |              |
| N7—H7D                | 0.91 (2)     | N7A—H7AD              | 0.91 (2)     |                       |              |
| C14—N1—N2             | 111.6 (5)    | C14A—N1A—N2A          | 110.6 (4)    |                       |              |
| C14—N1—C7             | 127.0 (5)    | C14A—N1A—C7A          | 126.9 (5)    |                       |              |
| N2—N1—C7              | 120.0 (5)    | N2A—N1A—C7A           | 120.5 (5)    |                       |              |
| C8—N2—N1              | 105.8 (5)    | C8A—N2A—N1A           | 106.4 (5)    |                       |              |
| C24—N3—N4             | 111.6 (5)    | C24A—N3A—N4A          | 111.5 (5)    |                       |              |
| C24—N3—C17            | 126.9 (5)    | C24A—N3A—C17A         | 127.3 (5)    |                       |              |
| N4—N3—C17             | 121.5 (5)    | N4A—N3A—C17A          | 121.1 (5)    |                       |              |
C18—N4—N3 105.6 (5)  C18A—N4A—N3A 106.3 (5)
N6—N5—C34 112.1 (6)  C34A—N5A—N6A 110.8 (5)
N6—N5—C27 122.3 (5)  C34A—N5A—C27A 128.2 (5)
C34—N5—C27 125.4 (6)  N6A—N5A—C27A 120.5 (5)
C6—C1—C2 121.0 (5)  C2A—C1A—C6A 121.1 (5)
C6—C1—C7 119.6 (5)  C2A—C1A—C7A 119.9 (5)
C2—C1—C7 119.4 (5)  C6A—C1A—C7A 119.1 (5)
C3—C2—C1 119.1 (5)  C1A—C2A—C3A 119.3 (5)
C3—C2—C15 120.6 (6)  C1A—C2A—C15A 120.1 (5)
C1—C2—C15 120.2 (5)  C3A—C2A—C15A 120.5 (5)
C2—C3—C4 120.8 (6)  C4A—C3A—C2A 120.9 (5)
C2—C3—C17 120.4 (5)  C4A—C3A—C17A 120.2 (5)
C4—C3—C17 118.8 (5)  C2A—C3A—C17A 118.9 (5)
C5—C4—C3 119.3 (5)  C5A—C4A—C3A 118.4 (5)
C5—C4—C25 120.6 (5)  C5A—C4A—C25A 121.0 (5)
C3—C4—C25 120.1 (5)  C3A—C4A—C25A 120.5 (6)
C4—C5—C6 121.0 (6)  C4A—C5A—C6A 121.9 (5)
C4—C5—C27 118.7 (6)  C4A—C5A—C27A 119.4 (5)
C6—C5—C27 120.3 (6)  C6A—C5A—C27A 118.7 (6)
C1—C6—C5 118.5 (6)  C5A—C6A—C1A 118.3 (6)
C1—C6—C35 120.7 (6)  C5A—C6A—C35A 121.4 (5)
C5—C6—C35 120.7 (5)  C1A—C6A—C35A 120.3 (5)
N1—C7—C1 112.3 (5)  N1A—C7A—C1A 112.2 (5)
N1—C7—H7E 109.1  N1A—C7A—H7AE 109.2
C1—C7—H7E 109.1  C1A—C7A—H7AE 109.2
N1—C7—H7F 109.1  N1A—C7A—H7AF 109.2
C1—C7—H7F 109.1  C1A—C7A—H7AF 109.2
H7E—C7—H7F 107.9  H7AE—C7A—H7AF 107.9
N2—C8—C9 111.6 (6)  N2A—C8A—C9A 111.5 (6)
N2—C8—H8 124.2  N2A—C8A—H8A 124.3
C9—C8—H8 124.2  C9A—C8A—H8A 124.3
C10—C9—C14 120.6 (6)  C10A—C9A—C14A 121.3 (6)
C10—C9—C8 135.2 (6)  C10A—C9A—C8A 134.5 (6)
C14—C9—C8 104.2 (5)  C14A—C9A—C8A 104.1 (5)
C11—C10—C9 115.6 (6)  C11A—C10A—C9A 115.6 (6)
C11—C10—C37 123.4 (6)  C11A—C10A—C37A 122.9 (6)
C9—C10—C37 120.9 (6)  C9A—C10A—C37A 121.5 (6)
C10—C11—C12 123.3 (6)  C10A—C11A—C12A 123.0 (6)
C10—C11—H11 118.4  C10A—C11A—H11A 118.5
C12—C11—H11 118.4  C12A—C11A—H11A 118.5
C13—C12—C11 121.3 (6)  C13A—C12A—C11A 121.4 (6)
C13—C12—H12 119.3  C13A—C12A—H12A 119.3
C11—C12—H12 119.3  C11A—C12A—H12A 119.3
C12—C13—C14 116.3 (6)  C12A—C13A—C14A 116.7 (6)
C12—C13—H13 121.8  C12A—C13A—H13A 121.7
C14—C13—H13 121.8  C14A—C13A—H13A 121.7
N1—C14—C13 130.5 (6)  N1A—C14A—C13A 130.7 (6)
| Bond                  | Distance (Å) | Bond                  | Distance (Å) |
|----------------------|--------------|----------------------|--------------|
| N1—C14—C9           | 106.8 (5)    | N1A—C14A—C9A        | 107.4 (5)    |
| C13—C14—C9          | 122.8 (6)    | C13A—C14A—C9A       | 122.0 (5)    |
| C2—C15—C16          | 111.5 (5)    | C2A—C15A—C16A       | 110.8 (5)    |
| C2—C15—H15A         | 109.3        | C2A—C15A—H15C       | 109.5        |
| C16—C15—H15A        | 109.3        | C16A—C15A—H15C      | 109.5        |
| C2—C15—H15B         | 109.3        | C2A—C15A—H15D       | 109.5        |
| C16—C15—H15B        | 109.3        | C16A—C15A—H15D      | 109.5        |
| H15A—C15—H15B       | 108.0        | H15C—C15A—H15D      | 108.1        |
| C15—C16—H16A        | 109.5        | C15A—C16A—H16D      | 109.5        |
| C15—C16—H16B        | 109.5        | C15A—C16A—H16E      | 109.5        |
| H16A—C16—H16B       | 109.5        | H16D—C16A—H16E      | 109.5        |
| C15—C16—H16C        | 109.5        | C15A—C16A—H16F      | 109.5        |
| H16A—C16—H16C       | 109.5        | H16D—C16A—H16F      | 109.5        |
| N3—C17—C3           | 111.3 (5)    | N3A—C17A—C3A        | 110.7 (5)    |
| N3—C17—H17A         | 109.4        | N3A—C17A—H17C       | 109.5        |
| C3—C17—H17A         | 109.4        | C3A—C17A—H17C       | 109.5        |
| N3—C17—H17B         | 109.4        | N3A—C17A—H17D       | 109.5        |
| C3—C17—H17B         | 109.4        | C3A—C17A—H17D       | 109.5        |
| H17A—C17—H17B       | 108.0        | H17C—C17A—H17D      | 108.1        |
| N4—C18—C19          | 111.4 (5)    | N4A—C18A—C19A       | 110.7 (5)    |
| N4—C18—H18          | 124.3        | N4A—C18A—H18A       | 124.6        |
| C19—C18—H18         | 124.3        | C19A—C18A—H18A      | 124.6        |
| C24—C19—C20         | 120.3 (5)    | C20A—C19A—C24A      | 120.4 (6)    |
| C24—C19—C18         | 104.9 (5)    | C20A—C19A—C18A      | 134.7 (6)    |
| C20—C19—C18         | 134.8 (6)    | C20A—C19A—C18A      | 104.9 (5)    |
| C21—C20—C19         | 116.6 (5)    | C21A—C20A—C19A      | 116.2 (6)    |
| C21—C20—C38         | 124.0 (6)    | C21A—C20A—C38A      | 124.5 (6)    |
| C19—C20—C38         | 119.4 (6)    | C19A—C20A—C38A      | 119.3 (6)    |
| C20—C21—C22         | 122.3 (6)    | C20A—C21A—C22A      | 122.9 (7)    |
| C20—C21—H21         | 118.9        | C20A—C21A—H21A      | 118.6        |
| C22—C21—H21         | 118.9        | C22A—C21A—H21A      | 118.6        |
| C23—C22—C21         | 121.9 (6)    | C23A—C22A—C21A      | 121.7 (7)    |
| C23—C22—H22         | 119.0        | C23A—C22A—H22A      | 119.2        |
| C21—C22—H22         | 119.0        | C21A—C22A—H22A      | 119.2        |
| C22—C23—C24         | 116.1 (6)    | C22A—C23A—C24A      | 116.0 (6)    |
| C22—C23—H23         | 121.9        | C22A—C23A—H23A      | 122.0        |
| C24—C23—H23         | 121.9        | C24A—C23A—H23A      | 122.0        |
| N3—C24—C23          | 130.7 (5)    | N3A—C24A—C23A       | 130.7 (6)    |
| N3—C24—C19          | 106.5 (5)    | N3A—C24A—C19A       | 106.5 (5)    |
| C23—C24—C19         | 122.8 (6)    | C23A—C24A—C19A      | 122.8 (6)    |
| C4—C25—C26          | 115.7 (5)    | C4A—C25A—C26A       | 115.1 (5)    |
| C4—C25—H25A         | 108.4        | C4A—C25A—H25C       | 108.5        |
| C26—C25—H25A        | 108.4        | C26A—C25A—H25C      | 108.5        |
| C4—C25—H25B         | 108.4        | C4A—C25A—H25D       | 108.5        |
| C26—C25—H25B        | 108.4        | C26A—C25A—H25D      | 108.5        |
| H25A—C25—H25B       | 107.4        | H25C—C25A—H25D      | 107.5        |
| C25—C26—H26A        | 109.5        | C25A—C26A—H26D      | 109.5        |
C25—C26—H26B 109.5  
H26A—C26—H26B 109.5  
C25—C26—H26C 109.5  
H26A—C26—H26C 109.5  
H26B—C26—H26C 109.5  
N5—C27—C5 113.7 (5)  
N5A—C27A—C5A 113.3 (5)  
N5—C27—H27A 108.8  
N5A—C27A—H27C 108.9  
C5—C27—H27A 108.8  
C5A—C27A—H27C 108.9  
C25—C26—H26C 109.5  
H26A—C26A—H26F 109.5  
H26B—C26A—H26F 109.5  
N5A—C27A—C5A 113.3 (5)  
N5A—C27A—H27C 108.9  
C5A—C27A—H27C 108.9  
N5—C27—H27A 108.8  
N5A—C27A—H27D 108.9  
C5—C27—H27A 108.8  
C5A—C27A—H27D 108.9  
H27A—C27—H27B 107.7  
H27C—C27A—H27D 107.7  
N6—C28—C29 111.2 (7)  
N6A—C28A—C29A 111.0 (5)  
N6—C28—H28 124.4  
N6A—C28A—H28A 124.5  
C29—C28—H28 124.4  
C29A—C28A—H28A 124.5  
C34—C29—C30 119.6 (7)  
C34A—C29A—C30A 121.0 (5)  
C34—C29—H29 124.4  
C34A—C29A—H29A 124.5  
C28—C29—C30 134.7 (8)  
C30A—C29A—C30A 123.6 (6)  
C29—C30—C39 126.3 (7)  
C31A—C30A—C39A 122.6 (6)  
C29—C30—H30 119.5 (8)  
C29A—C30A—H30A 120.8 (5)  
C31—C30—C39 114.2 (7)  
C31A—C30A—C39A 122.6 (6)  
C31—C30—C31 126.3 (7)  
C31A—C30A—C31A 122.0 (6)  
C32—C31—C30 119.5 (8)  
C32A—C31A—C30A 119.0  
C32—C31—H31 117.5  
C32A—C31A—H31A 119.0  
C30—C31—C30 129.1 (8)  
C30A—C31A—C30A 122.0  
C33—C32—C31 121.0 (8)  
C33A—C32A—C31A 122.2 (6)  
C33—C32—H32 119.5  
C33A—C32A—H32A 118.9  
C31—C32—C30 114.2 (7)  
C31A—C32A—C30A 118.9  
C31—C32—C33 126.3 (7)  
C31A—C32A—C33A 116.0 (6)  
C32—C33—C34 119.5  
C32A—C33A—C34A 122.0  
C32—C33—H33 121.9  
C32A—C33A—H33A 122.0  
N5—C34—C29 105.7 (6)  
N5A—C34A—C29A 107.5 (5)  
C34—C34—C33 119.5  
C34A—C33A—C34A 116.0 (6)  
C34—C34—C31 119.9  
C34A—C33A—C31A 118.9  
C34—C34—C29 123.6 (8)  
C34A—C33A—C29A 118.9  
C6—C35—C36 113.7 (5)  
C6A—C35A—C36A 113.5 (5)  
C6—C35—H35A 109.5  
C6A—C35A—H35C 108.9  
C36—C35—H35A 108.8  
C36A—C35A—H35C 108.9  
C6—C35—H35B 108.8  
C6A—C35A—H35D 108.9  
C36—C35—H35B 108.8  
C36A—C35A—H35D 108.9  
H35A—C35—H35B 107.7  
H35C—C35A—H35D 107.7  
C35—C36—H36A 109.5  
C35A—C36A—H36D 109.5  
C35—C36—H36B 109.5  
C35A—C36A—H36E 109.5  
H36A—C36—H36B 109.5  
H36D—C36A—H36E 109.5  
C35—C36—H36C 109.5  
C35A—C36A—H36F 109.5  
H36A—C36—H36C 109.5  
H36D—C36A—H36F 109.5  
C10—C37—H37A 109.5  
C10A—C37A—H37D 109.5  
C10—C37—H37B 109.5  
C10A—C37A—H37E 109.5  
H37A—C37—H37B 109.5  
H37D—C37A—H37E 109.5  
C10—C37—H37C 109.5  
C10A—C37A—H37F 109.5
H37A—C37—H37C 109.5  H37D—C37A—H37F 109.5
H37B—C37—H37C 109.5  H37E—C37A—H37F 109.5
C20—C38—H38A 109.5  C20A—C38A—H38D 109.5
C20—C38—H38B 109.5  C20A—C38A—H38E 109.5
H38A—C38—H38B 109.5  H38D—C38A—H38E 109.5
C20—C38—H38C 109.5  C20A—C38A—H38F 109.5
H38B—C38—H38C 109.5  H38E—C38A—H38F 109.5
C30—C39—H39A 109.5  C30A—C39A—H39D 109.5
C30—C39—H39B 109.5  C30A—C39A—H39E 109.5
H39A—C39—H39B 109.5  H39D—C39A—H39E 109.5
H39A—C39—H39C 109.5  H39D—C39A—H39F 109.5
H39B—C39—H39C 109.5  H39E—C39A—H39F 109.5
F4—P1—F1 89.9 (4)  F5A—P1A—F4A 89.6 (3)
F4—P1—F2 92.5 (5)  F5A—P1A—F6A 179.4 (3)
F1—P1—F2 176.9 (5)  F4A—P1A—F6A 89.8 (3)
F4—P1—F5 93.6 (3)  F5A—P1A—F1A 90.0 (2)
F1—P1—F5 90.6 (3)  F4A—P1A—F1A 90.8 (3)
F2—P1—F5 91.1 (4)  F6A—P1A—F1A 90.1 (2)
F4—P1—F3 179.5 (4)  F5A—P1A—F3A 90.7 (3)
F1—P1—F3 89.7 (4)  F4A—P1A—F3A 179.4 (3)
F2—P1—F3 87.9 (5)  F6A—P1A—F3A 89.9 (3)
F5—P1—F3 86.0 (3)  F1A—P1A—F3A 89.7 (2)
F4—P1—F6 89.0 (3)  F5A—P1A—F2A 90.1 (2)
F1—P1—F6 89.7 (3)  F4A—P1A—F2A 91.1 (2)
F2—P1—F6 88.5 (4)  F6A—P1A—F2A 89.8 (2)
F5—P1—F6 177.3 (3)  F1A—P1A—F2A 178.0 (3)
F3—P1—F6 91.3 (3)  F3A—P1A—F2A 88.4 (2)
H7C—N7—H7A 106 (9)  H7AD—N7A—H7AA 117 (8)
H7C—N7—H7D 109 (7)  H7AD—N7A—H7AB 109 (7)
H7A—N7—H7D 106 (8)  H7AA—N7A—H7AB 104 (8)
H7C—N7—H7B 111 (8)  H7AD—N7A—H7AC 108 (7)
H7A—N7—H7B 113 (8)  H7AA—N7A—H7AC 112 (9)
H7D—N7—H7B 111 (8)  H7AB—N7A—H7AC 105 (7)
C14—N1—N2—C8  −1.0 (7)  C14A—N1A—N2A—C8A  −1.5 (7)
C7—N1—N2—C8  −168.1 (6)  C7A—N1A—N2A—C8A  −166.5 (6)
C24—N3—N4—C18  0.3 (6)  C24A—N3A—N4A—C18A  0.1 (6)
C17—N3—N4—C18  −179.5 (5)  C17A—N3A—N4A—C18A  178.5 (5)
C34—N5—N6—C28  0.7 (8)  C34A—N5A—N6A—C28A  1.3 (7)
C27—N5—N6—C28  176.0 (6)  C27A—N5A—N6A—C28A  174.0 (6)
C6—C1—C2—C3  −3.1 (9)  C6A—C1A—C2A—C3A  −0.8 (9)
C7—C1—C2—C3  176.2 (5)  C7A—C1A—C2A—C3A  179.1 (5)
C6—C1—C2—C15  176.7 (5)  C6A—C1A—C2A—C15A  176.0 (5)
C7—C1—C2—C15  −4.0 (8)  C7A—C1A—C2A—C15A  −4.2 (8)
C1—C2—C3—C4  2.4 (8)  C1A—C2A—C3A—C4A  2.2 (9)
C15—C2—C3—C4  −177.4 (5)  C15A—C2A—C3A—C4A  −174.5 (5)
| Bond |  | Angles (deg) |  | Angles (deg) |
|------|---|-------------|---|-------------|
| C1—C2—C3—C17 | −176.6 (5) | C1A—C2A—C3A—C17A | −176.4 (5) |
| C15—C2—C3—C17 | 3.7 (8) | C15A—C2A—C3A—C17A | 6.9 (8) |
| C2—C3—C4—C5 | 1.9 (9) | C2A—C3A—C4A—C5A | −0.5 (8) |
| C17—C3—C4—C5 | −179.1 (5) | C17A—C3A—C4A—C5A | 178.1 (5) |
| C2—C3—C4—C25 | −174.9 (5) | C2A—C3A—C4A—C25A | 177.6 (5) |
| C17—C3—C4—C25 | 4.1 (8) | C17A—C3A—C4A—C25A | −3.9 (8) |
| C3—C4—C5—C6 | −5.6 (9) | C3A—C4A—C5A—C6A | −2.8 (9) |
| C25—C4—C5—C6 | 171.2 (5) | C25A—C4A—C5A—C6A | 179.2 (6) |
| C3—C4—C5—C27 | 173.8 (5) | C3A—C4A—C5A—C27A | 177.1 (5) |
| C25—C4—C5—C27 | −9.4 (9) | C25A—C4A—C5A—C27A | −1.0 (9) |
| C2—C1—C6—C5 | −0.4 (9) | C4A—C5A—C6A—C1A | 4.2 (9) |
| C7—C1—C6—C5 | −179.7 (5) | C27A—C5A—C6A—C1A | −175.7 (5) |
| C2—C1—C6—C35 | 176.1 (6) | C4A—C5A—C6A—C35A | −174.0 (6) |
| C7—C1—C6—C35 | −3.2 (8) | C27A—C5A—C6A—C35A | 6.2 (8) |
| C4—C5—C6—C1 | 4.9 (9) | C2A—C1A—C6A—C5A | −2.4 (8) |
| C27—C5—C6—C1 | −174.6 (5) | C7A—C1A—C6A—C5A | 177.8 (5) |
| C4—C5—C6—C35 | −171.7 (6) | C2A—C1A—C6A—C35A | 175.8 (5) |
| C27—C5—C6—C35 | 8.9 (9) | C7A—C1A—C6A—C35A | −4.0 (8) |
| C14—N1—C7—C1 | 149.3 (6) | C14A—N1A—C7A—C1A | 154.9 (6) |
| N2—N1—C7—C1 | −45.7 (8) | N2A—N1A—C7A—C1A | −42.8 (8) |
| C6—C1—C7—N1 | 100.0 (7) | C2A—C1A—C7A—N1A | −80.8 (7) |
| C2—C1—C7—N1 | −79.2 (7) | C6A—C1A—C7A—N1A | 99.0 (6) |
| N1—N2—C8—C9 | 0.1 (8) | N1A—N2A—C8A—C9A | 0.6 (7) |
| N2—C8—C9—C10 | −177.5 (7) | N2A—C8A—C9A—C10A | −179.2 (7) |
| C14—C9—C10—C11 | 2.0 (10) | C14A—C9A—C10A—C11A | 1.2 (9) |
| C8—C9—C10—C11 | −180.0 (7) | C8A—C9A—C10A—C11A | −179.0 (7) |
| C14—C9—C10—C37 | −177.8 (6) | C14A—C9A—C10A—C37A | −178.8 (6) |
| C8—C9—C10—C37 | 0.2 (12) | C8A—C9A—C10A—C37A | 1.0 (12) |
| C9—C10—C11—C12 | −0.9 (10) | C9A—C10A—C11A—C12A | 0.8 (9) |
| C37—C10—C11—C12 | 178.9 (7) | C37A—C10A—C11A—C12A | −179.3 (6) |
| C10—C11—C12—C13 | −0.3 (11) | C10A—C11A—C12A—C13A | −2.2 (10) |
| C11—C12—C13—C14 | 0.4 (10) | C11A—C12A—C13A—C14A | 1.5 (10) |
| N2—N1—C14—C13 | −179.2 (6) | N2A—N1A—C14A—C13A | −177.8 (6) |
| C7—N1—C14—C13 | −13.2 (11) | C7A—N1A—C14A—C13A | −14.0 (11) |
| N2—N1—C14—C9 | 1.4 (7) | N2A—N1A—C14A—C9A | 1.9 (7) |
| C7—N1—C14—C9 | 167.5 (6) | C7A—N1A—C14A—C9A | 165.7 (6) |
| C12—C13—C14—N1 | −178.5 (7) | C12A—C13A—C14A—N1A | −179.8 (6) |
| C11—C12—C13—C14 | 0.8 (9) | C12A—C13A—C14A—C9A | 0.5 (9) |
| C10—C9—C14—N1 | 177.3 (6) | C10A—C9A—C14A—N1A | 178.4 (6) |
| C8—C9—C14—N1 | −1.2 (7) | C8A—C9A—C14A—N1A | −1.5 (7) |
| C10—C9—C14—C13 | −2.1 (10) | C10A—C9A—C14A—C13A | −1.9 (10) |
| C8—C9—C14—C13 | 179.4 (6) | C8A—C9A—C14A—C13A | 178.3 (6) |
| C3—C2—C1—C15 | 85.0 (7) | C1A—C2A—C15A—C16A | −96.2 (7) |
| C1—C2—C15—C16 | −94.8 (7) | C3A—C2A—C15A—C16A | 80.5 (7) |
| C24—N3—C17—C3 | 154.5 (6) | C24A—N3A—C17A—C3A | 152.2 (6) |
| N4—N3—C17—C3 | −25.7 (7) | N4A—N3A—C17A—C3A | −25.9 (7) |
| C2—C3—C17—N3 | 98.7 (6) | C4A—C3A—C17A—N3A | −78.8 (7) |
| Bond          | Angle (deg) | Bond          | Angle (deg) |
|--------------|-------------|--------------|-------------|
| C4—C3—C17—N3 | -80.2 (7)   | C2A—C3A—C17A—N3A | 99.8 (6)   |
| N3—N4—C18—C19 | -0.3 (7)    | N3A—N4A—C18A—C19A | -0.4 (6)   |
| N4—C18—C19—C20 | 0.3 (7)     | N4A—C18A—C19A—C20A | -178.7 (7) |
| N4—C18—C19—C20 | -177.3 (6)  | N4A—C18A—C19A—C20A | 0.6 (7)    |
| C24—C19—C20—C21 | 0.0 (9)     | C24A—C19A—C20A—C21A | -0.1 (9)   |
| C18—C19—C20—C21 | 177.2 (7)   | C18A—C19A—C20A—C21A | 179.1 (7)  |
| C24—C19—C20—C21 | -178.4 (6)  | C24A—C19A—C20A—C21A | -179.8 (6) |
| C18—C19—C20—C21 | -1.2 (11)   | C18A—C19A—C20A—C21A | -0.6 (11)  |
| C19—C20—C21—C22 | 0.6 (9)     | C19A—C20A—C21A—C22A | 0.6 (10)   |
| C38—C20—C21—C22 | 179.0 (6)   | C38A—C20A—C21A—C22A | -179.7 (7) |
| C20—C21—C22—C23 | -0.5 (10)   | C20A—C21A—C22A—C23A | 0.0 (11)   |
| C21—C22—C23—C24 | -0.2 (9)    | C21A—C22A—C23A—C24A | -1.0 (10)  |
| N4—N3—C24—C23 | 178.4 (6)   | N4A—N3A—C24A—C23A | -180.0 (6) |
| C17—N3—C24—C23 | -1.9 (11)   | C17A—N3A—C24A—C23A | 1.9 (11)   |
| N4—N3—C24—C19 | -0.1 (7)    | N4A—N3A—C24A—C19A | 0.2 (7)    |
| C17—N3—C24—C19 | 179.6 (5)   | C17A—N3A—C24A—C19A | -178.0 (5) |
| C18—C19—C20—C21 | 177.9 (5)   | C18A—C19A—C20A—C21A | 1.4 (9)    |
| C20—C19—C20—C21 | -0.7 (9)    | C20A—C19A—C20A—C21A | 0.9 (9)    |
| C18—C19—C20—C21 | -178.7 (6)  | C18A—C19A—C20A—C21A | 179.7 (6)  |
| C5—C4—C25—C26 | 93.7 (7)    | C5A—C4A—C25A—C26A | -91.4 (7)  |
| C3—C4—C25—C26 | -89.6 (7)   | C3A—C4A—C25A—C26A | 90.5 (7)   |
| N6—N5—C27—C5 | 27.5 (9)    | N6A—N5A—C27A—C5A | -149.0 (6) |
| C34—N5—C27—C5 | -157.8 (6)  | N6A—N5A—C27A—C5A | 39.8 (8)   |
| C4—C5—C27—N5 | 79.7 (8)    | C4A—C5A—C27A—N5A | 75.9 (7)   |
| C6—C5—C27—N5 | -100.9 (7)  | C6A—C5A—C27A—N5A | -104.3 (7) |
| N5—N6—C28—C29 | -1.0 (9)    | N5A—N6A—C28A—C29A | -1.5 (7)   |
| N6—C28—C29—C34 | 0.9 (9)     | N6A—C28A—C29A—C34A | 1.2 (7)    |
| N6—C28—C29—C30 | -179.3 (8)  | N6A—C28A—C29A—C30A | -179.5 (7) |
| C34—C29—C30—C31 | 0.3 (10)    | C34A—C29A—C30A—C31A | -0.1 (9)   |
| C28—C29—C30—C31 | -179.4 (8)  | C28A—C29A—C30A—C31A | -179.4 (7) |
| C34—C29—C30—C31 | 179.7 (7)   | C34A—C29A—C30A—C31A | 179.3 (6)  |
| C28—C29—C30—C31 | 0.0 (13)    | C28A—C29A—C30A—C31A | 0.0 (11)   |
| C29—C30—C31—C32 | 2.4 (12)    | C29A—C30A—C31A—C32A | 1.6 (9)    |
| C39—C30—C31—C32 | -177.0 (8)  | C39A—C30A—C31A—C32A | -177.8 (7) |
| C30—C31—C32—C33 | -3.9 (13)   | C30A—C31A—C32A—C33A | -1.7 (10)  |
| C31—C32—C33—C34 | 2.3 (12)    | C31A—C32A—C33A—C34A | 0.1 (10)   |
| N6—N5—C34—C29 | -0.1 (8)    | N6A—N5A—C34A—C29A | -0.6 (7)   |
| C27—N5—C34—C29 | -175.3 (6)  | C27A—N5A—C34A—C29A | -172.6 (6) |
| N6—N5—C34—C33 | -178.5 (8)  | N6A—N5A—C34A—C33A | -178.8 (6) |
| C27—N5—C34—C33 | 6.3 (12)    | C27A—N5A—C34A—C33A | 9.3 (11)   |
| C28—C29—C34—N5 | -0.5 (8)    | C30A—C29A—C34A—N5A | -179.8 (6) |
| C30—C29—C34—N5 | 179.7 (6)   | C28A—C29A—C34A—N5A | -0.3 (7)   |
| C28—C29—C34—N5 | 178.1 (7)   | C30A—C29A—C34A—N5A | -1.5 (9)   |
| C30—C29—C34—N5 | -1.7 (11)   | C28A—C29A—C34A—C33A | 178.0 (6)  |
| C32—C33—C34—N5 | 178.6 (7)   | C32A—C33A—C34A—N5A | 179.3 (6)  |
Hydrogen-bond geometry (Å, °)

Cg1, Cg2 and Cg3 represent the centroids of the N3/N4/C18/C19/C24, N3A/N4A/C18A/C19A/C24A and N5A/N6A/C28A/C29A/C34A rings, respectively.

| D—H···A          | D—H | H···A | D···A | D—H···A |
|------------------|-----|-------|-------|---------|
| N7—H7A···N2i     | 0.91 (2) | 2.02 (3) | 2.923 (8) | 171 (9) |
| N7—H7B···N4i     | 0.91 (2) | 2.10 (4) | 2.980 (8) | 162 (8) |
| N7—H7C···N6i     | 0.91 (2) | 2.01 (2) | 2.923 (9) | 175 (9) |
| N7—H7D···F3      | 0.91 (2) | 2.06 (3) | 2.951 (8) | 164 (7) |
| N7—H7D···F5      | 0.91 (2) | 2.54 (6) | 3.213 (8) | 131 (6) |
| C13—H13···F6A    | 0.95  | 2.55   | 3.500 (9) | 176    |
| C17—H17A···F1    | 0.99  | 2.52   | 3.156 (7) | 117    |
| C18—H18···F2A    | 0.95  | 2.33   | 3.201 (8) | 151    |
| C22—H22···F5A    | 0.95  | 2.45   | 3.325 (8) | 154    |
| C23—H23···F4     | 0.95  | 2.60   | 3.552 (8) | 175    |
| C31—H31···F3B    | 0.95  | 2.35   | 3.289 (8) | 173    |
| C37—H37C···F2A   | 0.98  | 2.51   | 3.379 (9) | 148    |
| N7A—H7AA···N2A   | 0.91 (2) | 2.02 (3) | 2.917 (8) | 171 (10) |
| N7A—H7AB···N4A   | 0.91 (2) | 2.09 (3) | 2.969 (8) | 161 (8) |
| N7A—H7AC···N6A   | 0.92 (2) | 2.03 (3) | 2.941 (7) | 172 (8) |
| N7A—H7AD···F3A   | 0.91 (2) | 2.17 (3) | 3.050 (7) | 164 (6) |
| N7A—H7AD···F2A   | 0.91 (2) | 2.43 (6) | 3.096 (7) | 130 (6) |
| C17A—H17D···F1A  | 0.99  | 2.59   | 3.247 (7) | 124    |
| C18A—H18A···F6A  | 0.95  | 2.44   | 3.317 (8) | 154    |
| C23A—H23A···F4A  | 0.95  | 2.61   | 3.561 (8) | 177    |
| C36A—H36B···Cg2  | 0.98  | 2.77   | 3.481 (7) | 130    |
| C26A—H26E···Cg3  | 0.98  | 2.66   | 3.592 (7) | 158    |
| C26A—H26F···Cg2  | 0.98  | 2.56   | 3.506 (7) | 163    |
| C36A—H36F···Cg1  | 0.98  | 2.82   | 3.605 (7) | 138    |

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