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3-Chloro-6-nitro-1-[(1-octyl-1*H*-1,2,3-triazol-4-yl)-methyl]-1*H*-indazole

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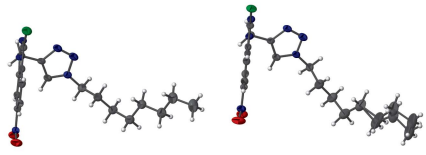
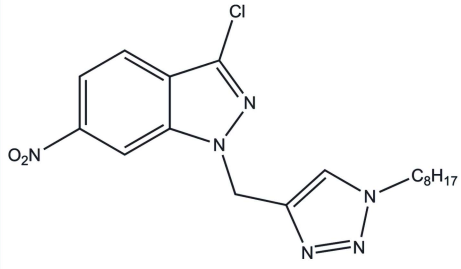
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title compound, $C_{18}H_{23}ClN_6O_2$, consists of two independent molecules differing primarily in the dihedral angles between the mean planes of the indazole and triazole moieties [78.50 (8) in one and 72.39 (7)° in the other]. One of the molecules shows positional disorder of the terminal part of its octyl chain. In the crystal, C—H···X (X = Cl, N, O) hydrogen bonds and C—H···π and π-stacking interactions are observed: together these generate a three-dimensional network.

3D view



Chemical scheme



Structure description

As a continuation of our studies of indazole derivatives (Boulhaoua *et al.*, 2016), we report the synthesis and structure of the title compound.

The asymmetric unit of the title compound consists of two independent molecules having very similar conformations and so an ellipsoid plot of only one molecule is shown (Fig. 1). The primary differences between the two are a disorder in the C34–C35–C36 portion of one alkyl chain and different dihedral angles between the mean planes of the indazole and triazole rings, being 78.50 (8)° in the molecule containing Cl1 and 72.39 (7)° in the other.

As shown in Fig. 2, there are a number of different intermolecular interactions. The C—H···X (X = Cl, N, O) hydrogen bonds as well as the C—H···π(ring) interactions are listed in Table 1. In addition there are π–π stacking interactions between centrosymmetrically related indazole units [$Cg1\cdots Cg3$ = 3.636 (2) Å, dihedral angle 0.53 (14)°]. The result is a three-dimensional supramolecular network (Fig. 3) in which the long alkyl chains tend to intercalate but the segregation of 'head' and 'tail' portions is not as pronounced as in related molecules (Boulhaoua *et al.*, 2016).

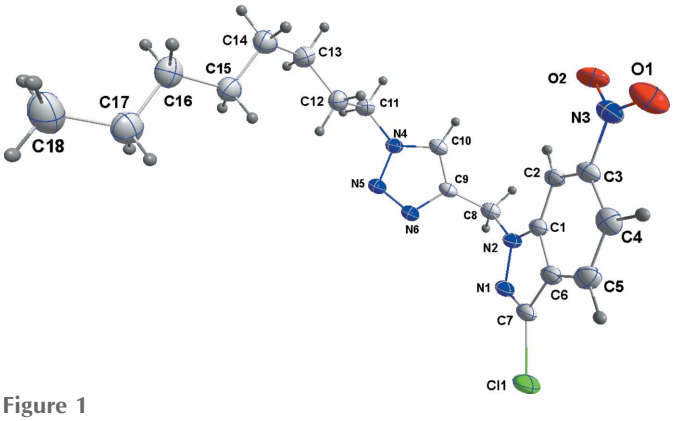


Figure 1
The C1 molecule showing 50% probability ellipsoids.

Synthesis and crystallization

To a solution of 3-chloro-6-nitro-1-(prop-2-yn-1-yl)-1*H*-indazole (0.3 g, 1.27 mmol) in ethanol (15 ml) was added 1-azidooctane (0.24 g, 1.53 mmol). The mixture was stirred under reflux for 48 h. After completion of reaction (monitored by TLC), the solution was concentrated and the residue was purified by column chromatography on silica gel by using a mixture (hexane/ethyl acetate 9/1). Crystals were obtained when the solvent was allowed to evaporate. The solid product was purified by recrystallization from ethanol solution to afford colourless crystals in 70% yield.

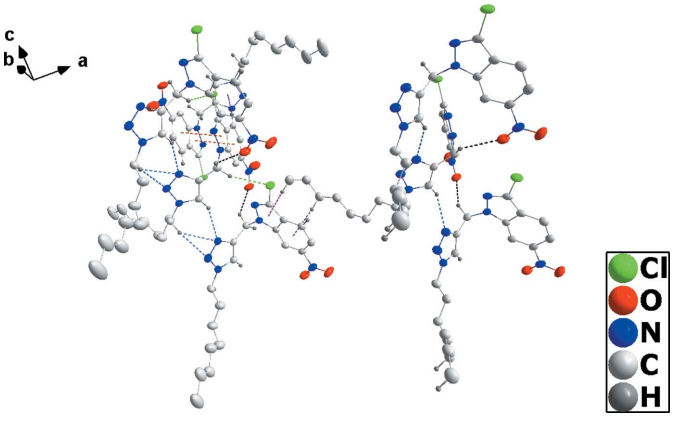


Figure 2
Detail of the intermolecular interactions [dotted lines: C—H···O, black; C—H···N, blue; C—H···Cl, green; C—H···π(ring), purple, π-stacking, orange].

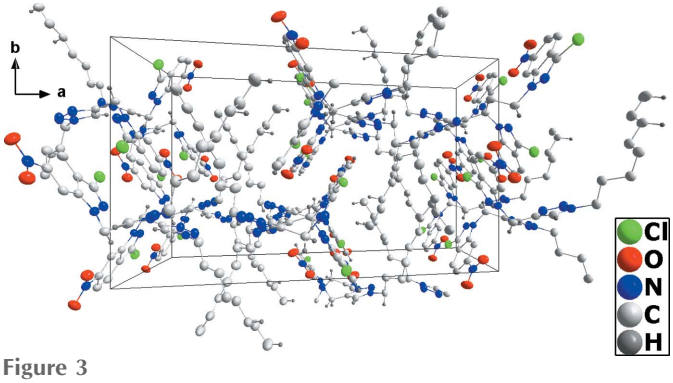


Figure 3
Packing viewed along the *c* axis.

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

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the N7/N8/C19/C24/C25, N10/N11/N12/C27/C28 and C19–C24 rings, respectively

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8A···O2^{i}	0.98 (3)	2.62 (3)	3.348 (3)	132 (2)
C10—H10···N6^{ii}	0.93 (3)	2.57 (3)	3.377 (3)	145 (2)
C26—H26A···O4^{iii}	0.95 (3)	2.54 (3)	3.240 (3)	131 (2)
C26—H26B···Cl2^{iv}	0.98 (3)	2.82 (3)	3.682 (3)	147 (2)
C28—H28···N12^{iv}	0.92 (3)	2.45 (3)	3.298 (3)	152 (2)
C29—H29B···N11^{iv}	1.05 (3)	2.63 (3)	3.594 (4)	153 (2)
C29—H29B···N12^{iv}	1.05 (3)	2.65 (3)	3.476 (3)	135 (2)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{23}ClN_6O_2$
M_r	390.87
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	150
a, b, c (Å)	25.3512 (9), 14.9091 (5), 10.7525 (3)
β (°)	101.725 (2)
V (Å^3)	3979.3 (2)
Z	8
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.91
Crystal size (mm)	0.12 × 0.12 × 0.02
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.80, 0.96
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22444, 7460, 5327
R_{int}	0.068
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.610
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.058, 0.117, 1.09
No. of reflections	7460
No. of parameters	653
No. of restraints	10
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.19, −0.28

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Carbon atoms C34–C36 are disordered over two closely spaced sites in a 0.52 (2):0.48 (2) ratio. The components of the disorder were refined subject to restraints that their geometries approximate that of the corresponding portion of the ordered alkyl chain. The

hydrogen atoms attached to the disordered atoms were included as riding contributions in idealized positions. Trial refinements with the single-component data extracted from the full data set with *TWINABS* (Sheldrick, 2009) and with the full three-component data indicated that the former refinement was superior.

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x170146 [https://doi.org/10.1107/S2414314617001468]

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Crystal data

$C_{18}H_{23}ClN_6O_2$
M_r = 390.87
Monoclinic, $P2_1/c$
a = 25.3512 (9) Å
b = 14.9091 (5) Å
c = 10.7525 (3) Å
β = 101.725 (2)°
V = 3979.3 (2) Å^3
Z = 8
$F(000)$ = 1648
D_x = 1.305 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9411 reflections
θ = 3.6–70.1°
μ = 1.91 mm^{-1}
T = 150 K
Plate, colourless
0.12 × 0.12 × 0.02 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro-focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.80, T_{max} = 0.96
22444 measured reflections
7460 independent reflections
5327 reflections with $I > 2\sigma(I)$
R_{int} = 0.068
θ_{max} = 70.2°, θ_{min} = 3.5°
h = −30→30
k = −17→18
l = −13→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.117
S = 1.09
7460 reflections
653 parameters
10 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0372P)^2 + 1.7954P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Special details

Experimental. Analysis of 2946 reflections having I/σ(I) > 12 and chosen from the full data set with *CELL_NOW* (Sheldrick, 2008) showed the crystal to belong to the monoclinic system and to consist of at least three components. With approximately 90% of the reflections indexed with the three major components, it was decided to use these for the structure determination. The raw data were processed using the multi-component version of *SAINT* under control of the three-component orientation file generated by *CELL_NOW*.

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger. Carbons C34-C36 are disordered over two closely spaced sites in a 52:48 ratio. The components of the disorder were refined subject to restraints that their geometries approximate that of the corresponding portion of the ordered alkyl chain. The hydrogen atoms attached to the disordered atoms were included as riding contributions in idealized positions. Trial refinements with the single-component data extracted from the full data set with *TWINABS* and with the full 3-component data indicated that the former refinement was superior.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cl1	1.06482 (3)	−0.05492 (5)	0.71585 (6)	0.0410 (2)	
O1	1.08776 (9)	0.06599 (14)	0.0520 (2)	0.0495 (6)	
O2	1.04771 (9)	−0.05912 (13)	−0.00830 (17)	0.0420 (5)	
N1	1.02266 (9)	−0.17337 (15)	0.54180 (19)	0.0297 (5)	
N2	1.01686 (9)	−0.18696 (14)	0.41414 (19)	0.0261 (5)	
N3	1.06707 (9)	−0.00487 (16)	0.0742 (2)	0.0332 (6)	
N4	0.85290 (9)	−0.19184 (14)	0.17346 (19)	0.0289 (5)	
N5	0.84521 (10)	−0.18829 (17)	0.2940 (2)	0.0377 (6)	
N6	0.89099 (10)	−0.21181 (16)	0.3684 (2)	0.0350 (6)	
C1	1.03835 (10)	−0.11787 (16)	0.3578 (2)	0.0238 (6)	
C2	1.04026 (10)	−0.10374 (17)	0.2305 (2)	0.0254 (6)	
H2	1.0265 (10)	−0.1453 (18)	0.163 (2)	0.032 (7)*	
C3	1.06481 (11)	−0.02509 (17)	0.2070 (2)	0.0272 (6)	
C4	1.08714 (11)	0.03768 (19)	0.3007 (3)	0.0311 (6)	
H4	1.1042 (11)	0.0894 (19)	0.274 (3)	0.038 (8)*	
C5	1.08466 (11)	0.02235 (19)	0.4247 (3)	0.0312 (6)	
H5	1.0981 (11)	0.0650 (18)	0.487 (3)	0.031 (7)*	
C6	1.05969 (10)	−0.05621 (17)	0.4539 (2)	0.0262 (6)	
C7	1.04850 (11)	−0.09668 (18)	0.5652 (2)	0.0288 (6)	
C8	0.98327 (11)	−0.25993 (18)	0.3518 (3)	0.0295 (6)	
H8A	0.9824 (11)	−0.3072 (19)	0.415 (3)	0.040 (8)*	
H8B	1.0020 (11)	−0.2874 (17)	0.289 (3)	0.036 (8)*	
C9	0.92765 (10)	−0.23026 (16)	0.2950 (2)	0.0256 (6)	
C10	0.90359 (11)	−0.21735 (17)	0.1714 (2)	0.0289 (6)	
H10	0.9156 (11)	−0.2263 (18)	0.096 (3)	0.040 (8)*	
C11	0.80896 (12)	−0.1697 (2)	0.0677 (3)	0.0350 (7)	
H11A	0.7751 (12)	−0.2037 (19)	0.081 (3)	0.043 (8)*	

H11B	0.8189 (10)	−0.1895 (17)	−0.014 (3)	0.033 (7)*
C12	0.79522 (12)	−0.0710 (2)	0.0601 (3)	0.0356 (7)
H12A	0.8262 (12)	−0.037 (2)	0.050 (3)	0.045 (9)*
H12B	0.7866 (11)	−0.0526 (18)	0.143 (3)	0.038 (8)*
C13	0.74781 (13)	−0.0525 (2)	−0.0495 (3)	0.0376 (7)
H13A	0.7182 (12)	−0.091 (2)	−0.033 (3)	0.045 (9)*
H13B	0.7571 (12)	−0.0748 (19)	−0.135 (3)	0.049 (9)*
C14	0.73000 (14)	0.0451 (2)	−0.0636 (3)	0.0412 (7)
H14A	0.7609 (13)	0.084 (2)	−0.085 (3)	0.052 (9)*
H14B	0.6973 (13)	0.050 (2)	−0.137 (3)	0.053 (9)*
C15	0.71683 (13)	0.0848 (2)	0.0577 (3)	0.0400 (7)
H15A	0.6948 (12)	0.036 (2)	0.098 (3)	0.055 (9)*
H15B	0.7512 (13)	0.094 (2)	0.123 (3)	0.058 (10)*
C16	0.68594 (13)	0.1729 (2)	0.0359 (3)	0.0414 (7)
H16A	0.6491 (11)	0.1608 (18)	−0.026 (3)	0.035 (8)*
H16B	0.7052 (13)	0.219 (2)	−0.011 (3)	0.054 (9)*
C17	0.67661 (14)	0.2152 (2)	0.1587 (3)	0.0484 (8)
H17A	0.6599 (12)	0.169 (2)	0.205 (3)	0.044 (9)*
H17B	0.7125 (14)	0.229 (2)	0.219 (3)	0.056 (10)*
C18	0.64275 (17)	0.2996 (2)	0.1374 (4)	0.0583 (10)
H18A	0.6599 (16)	0.351 (3)	0.089 (4)	0.089 (13)*
H18B	0.6072 (16)	0.289 (2)	0.078 (4)	0.078 (13)*
H18C	0.6357 (17)	0.325 (3)	0.218 (4)	0.104 (15)*
Cl2	0.56098 (3)	0.42012 (5)	0.81890 (6)	0.03704 (19)
O3	0.59263 (10)	0.54356 (14)	0.16175 (19)	0.0541 (6)
O4	0.53884 (9)	0.43426 (13)	0.09351 (17)	0.0422 (5)
N7	0.51073 (9)	0.31204 (14)	0.63903 (19)	0.0279 (5)
N8	0.50277 (8)	0.30233 (14)	0.50996 (18)	0.0253 (5)
N9	0.56383 (10)	0.48075 (15)	0.1790 (2)	0.0343 (6)
N10	0.33838 (9)	0.29026 (14)	0.26015 (19)	0.0275 (5)
N11	0.33042 (10)	0.29952 (16)	0.3790 (2)	0.0347 (6)
N12	0.37630 (9)	0.28032 (15)	0.45646 (19)	0.0304 (5)
C19	0.52779 (10)	0.36914 (16)	0.4569 (2)	0.0237 (6)
C20	0.53062 (11)	0.38525 (18)	0.3310 (2)	0.0262 (6)
H20	0.5130 (10)	0.3491 (16)	0.264 (2)	0.022 (7)*
C21	0.55916 (11)	0.46036 (17)	0.3111 (2)	0.0266 (6)
C22	0.58479 (11)	0.51830 (18)	0.4076 (2)	0.0274 (6)
H22	0.6046 (11)	0.5697 (19)	0.388 (3)	0.038 (8)*
C23	0.58208 (11)	0.50056 (18)	0.5310 (2)	0.0268 (6)
H23	0.5977 (10)	0.5392 (16)	0.594 (2)	0.021 (7)*
C24	0.55317 (10)	0.42522 (17)	0.5560 (2)	0.0246 (6)
C25	0.54078 (10)	0.38417 (17)	0.6656 (2)	0.0260 (6)
C26	0.46897 (11)	0.22959 (18)	0.4453 (3)	0.0283 (6)
H26A	0.4689 (11)	0.1842 (19)	0.507 (3)	0.042 (8)*
H26B	0.4874 (11)	0.2060 (17)	0.380 (3)	0.032 (7)*
C27	0.41350 (10)	0.25869 (16)	0.3862 (2)	0.0244 (6)
C28	0.38949 (11)	0.26531 (18)	0.2614 (2)	0.0289 (6)
H28	0.3989 (11)	0.2544 (17)	0.184 (3)	0.034 (7)*

C29	0.29440 (12)	0.3054 (2)	0.1510 (3)	0.0321 (6)	
H29A	0.2593 (13)	0.295 (2)	0.177 (3)	0.063 (10)*	
H29B	0.3003 (11)	0.2555 (19)	0.086 (3)	0.042 (8)*	
C30	0.29403 (14)	0.3990 (2)	0.0970 (3)	0.0419 (8)	
H30A	0.2884 (13)	0.444 (2)	0.159 (3)	0.058 (10)*	
H30B	0.3310 (12)	0.4134 (18)	0.073 (3)	0.038 (8)*	
C31	0.24855 (14)	0.4069 (2)	−0.0213 (3)	0.0468 (8)	
H31A	0.2146 (15)	0.385 (2)	0.001 (3)	0.069 (11)*	
H31B	0.2576 (13)	0.364 (2)	−0.094 (3)	0.062 (10)*	
C32	0.24006 (16)	0.5007 (2)	−0.0759 (4)	0.0534 (9)	
H32A	0.2791 (15)	0.523 (2)	−0.103 (3)	0.075 (11)*	
H32B	0.2112 (16)	0.500 (2)	−0.159 (4)	0.080 (12)*	
C33	0.22209 (16)	0.5683 (2)	0.0135 (4)	0.0559 (9)	
H33A	0.1953 (14)	0.535 (2)	0.064 (3)	0.072 (11)*	
H33B	0.2549 (15)	0.586 (2)	0.089 (4)	0.078 (12)*	
C34A	0.1940 (16)	0.6549 (15)	−0.0388 (19)	0.056 (3)	0.52 (2)
H34A	0.2176	0.6867	−0.0873	0.068*	0.52 (2)
H34B	0.1604	0.6389	−0.0995	0.068*	0.52 (2)
C35A	0.1797 (11)	0.7196 (13)	0.0590 (17)	0.066 (3)	0.52 (2)
H35A	0.1592	0.6867	0.1137	0.079*	0.52 (2)
H35B	0.2134	0.7417	0.1138	0.079*	0.52 (2)
C36A	0.1466 (8)	0.7993 (10)	0.000 (2)	0.087 (5)	0.52 (2)
H36A	0.1388	0.8382	0.0678	0.130*	0.52 (2)
H36B	0.1670	0.8332	−0.0523	0.130*	0.52 (2)
H36C	0.1128	0.7782	−0.0524	0.130*	0.52 (2)
C34B	0.1972 (17)	0.6467 (17)	−0.069 (2)	0.056 (3)	0.48 (2)
H34C	0.2249	0.6747	−0.1097	0.068*	0.48 (2)
H34D	0.1679	0.6244	−0.1374	0.068*	0.48 (2)
C35B	0.1749 (12)	0.7166 (15)	0.0098 (17)	0.066 (3)	0.48 (2)
H35C	0.1484	0.6874	0.0527	0.079*	0.48 (2)
H35D	0.2046	0.7396	0.0764	0.079*	0.48 (2)
C36B	0.1480 (9)	0.7950 (11)	−0.068 (2)	0.087 (5)	0.48 (2)
H36D	0.1345	0.8374	−0.0123	0.130*	0.48 (2)
H36E	0.1742	0.8252	−0.1093	0.130*	0.48 (2)
H36F	0.1178	0.7730	−0.1329	0.130*	0.48 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0475 (5)	0.0555 (5)	0.0194 (3)	0.0032 (4)	0.0054 (3)	−0.0071 (3)
O1	0.0690 (16)	0.0420 (13)	0.0445 (13)	−0.0062 (11)	0.0281 (11)	0.0091 (10)
O2	0.0612 (15)	0.0426 (13)	0.0248 (10)	0.0021 (10)	0.0150 (10)	−0.0014 (9)
N1	0.0326 (14)	0.0387 (14)	0.0182 (11)	0.0047 (10)	0.0064 (10)	0.0010 (10)
N2	0.0313 (13)	0.0288 (12)	0.0186 (11)	−0.0016 (10)	0.0057 (9)	0.0004 (9)
N3	0.0377 (15)	0.0358 (14)	0.0296 (13)	0.0102 (11)	0.0149 (11)	0.0077 (11)
N4	0.0318 (14)	0.0329 (13)	0.0222 (11)	−0.0010 (10)	0.0062 (10)	−0.0010 (9)
N5	0.0368 (15)	0.0553 (16)	0.0226 (12)	−0.0002 (12)	0.0097 (11)	−0.0026 (11)
N6	0.0363 (15)	0.0466 (15)	0.0237 (12)	0.0001 (11)	0.0101 (11)	−0.0014 (10)

C1	0.0254 (15)	0.0253 (14)	0.0209 (13)	0.0025 (11)	0.0049 (11)	−0.0001 (11)
C2	0.0287 (15)	0.0271 (15)	0.0210 (13)	0.0055 (11)	0.0068 (11)	−0.0014 (11)
C3	0.0321 (16)	0.0280 (15)	0.0233 (13)	0.0063 (12)	0.0101 (12)	0.0034 (11)
C4	0.0319 (17)	0.0289 (15)	0.0336 (15)	0.0032 (12)	0.0092 (13)	0.0024 (12)
C5	0.0320 (17)	0.0290 (16)	0.0313 (15)	0.0025 (12)	0.0034 (13)	−0.0082 (13)
C6	0.0269 (15)	0.0304 (15)	0.0212 (13)	0.0060 (11)	0.0045 (11)	−0.0023 (11)
C7	0.0294 (16)	0.0381 (16)	0.0190 (13)	0.0077 (12)	0.0050 (11)	−0.0018 (11)
C8	0.0382 (17)	0.0253 (15)	0.0263 (14)	0.0003 (12)	0.0094 (13)	0.0001 (12)
C9	0.0343 (16)	0.0231 (13)	0.0215 (13)	−0.0024 (11)	0.0108 (12)	0.0002 (11)
C10	0.0361 (17)	0.0292 (15)	0.0240 (14)	−0.0008 (12)	0.0120 (12)	−0.0006 (11)
C11	0.0355 (18)	0.0412 (18)	0.0271 (15)	0.0029 (14)	0.0034 (13)	−0.0023 (13)
C12	0.0325 (18)	0.0405 (18)	0.0337 (16)	−0.0003 (14)	0.0067 (13)	0.0020 (13)
C13	0.0388 (19)	0.0395 (18)	0.0334 (16)	0.0008 (14)	0.0044 (14)	0.0028 (13)
C14	0.039 (2)	0.0444 (19)	0.0408 (18)	0.0004 (15)	0.0092 (16)	0.0059 (15)
C15	0.0365 (19)	0.0447 (19)	0.0383 (17)	0.0018 (15)	0.0068 (15)	0.0027 (14)
C16	0.0348 (19)	0.0390 (19)	0.050 (2)	−0.0025 (14)	0.0077 (16)	0.0006 (15)
C17	0.040 (2)	0.052 (2)	0.052 (2)	0.0006 (16)	0.0043 (17)	−0.0060 (17)
C18	0.053 (3)	0.049 (2)	0.072 (3)	0.0042 (19)	0.011 (2)	−0.017 (2)
Cl2	0.0440 (4)	0.0484 (4)	0.0182 (3)	−0.0063 (3)	0.0051 (3)	−0.0048 (3)
O3	0.0823 (18)	0.0465 (13)	0.0381 (12)	−0.0204 (12)	0.0230 (12)	0.0045 (10)
O4	0.0610 (15)	0.0438 (13)	0.0227 (10)	−0.0034 (10)	0.0107 (10)	−0.0030 (9)
N7	0.0299 (13)	0.0349 (13)	0.0181 (11)	0.0030 (10)	0.0034 (9)	−0.0009 (9)
N8	0.0286 (13)	0.0281 (12)	0.0185 (10)	−0.0006 (9)	0.0032 (9)	−0.0006 (9)
N9	0.0481 (16)	0.0316 (13)	0.0261 (12)	0.0028 (11)	0.0140 (12)	0.0012 (11)
N10	0.0284 (13)	0.0343 (13)	0.0200 (11)	−0.0004 (10)	0.0058 (10)	−0.0027 (9)
N11	0.0373 (15)	0.0448 (15)	0.0240 (12)	−0.0020 (11)	0.0108 (11)	−0.0047 (10)
N12	0.0304 (14)	0.0406 (14)	0.0209 (11)	−0.0043 (10)	0.0067 (10)	−0.0013 (10)
C19	0.0213 (14)	0.0259 (14)	0.0234 (13)	0.0055 (11)	0.0033 (11)	0.0005 (11)
C20	0.0285 (16)	0.0288 (15)	0.0203 (13)	0.0040 (12)	0.0022 (12)	−0.0030 (11)
C21	0.0333 (16)	0.0274 (14)	0.0204 (13)	0.0060 (12)	0.0087 (11)	0.0019 (11)
C22	0.0286 (16)	0.0245 (15)	0.0302 (14)	0.0006 (12)	0.0088 (12)	0.0011 (12)
C23	0.0265 (16)	0.0287 (15)	0.0246 (14)	0.0018 (11)	0.0040 (12)	−0.0047 (12)
C24	0.0241 (15)	0.0279 (14)	0.0217 (13)	0.0041 (11)	0.0044 (11)	−0.0012 (11)
C25	0.0291 (15)	0.0329 (15)	0.0158 (12)	0.0028 (12)	0.0041 (11)	−0.0005 (11)
C26	0.0333 (16)	0.0254 (15)	0.0256 (14)	−0.0007 (12)	0.0042 (12)	−0.0020 (12)
C27	0.0319 (16)	0.0205 (13)	0.0222 (13)	−0.0026 (11)	0.0086 (11)	−0.0002 (10)
C28	0.0319 (17)	0.0351 (16)	0.0208 (14)	−0.0004 (12)	0.0079 (12)	−0.0014 (12)
C29	0.0265 (17)	0.0405 (17)	0.0280 (15)	0.0034 (13)	0.0027 (12)	−0.0005 (13)
C30	0.046 (2)	0.0394 (19)	0.0379 (18)	0.0046 (15)	0.0015 (15)	0.0012 (14)
C31	0.048 (2)	0.049 (2)	0.0387 (18)	0.0039 (17)	−0.0029 (16)	0.0066 (16)
C32	0.055 (2)	0.050 (2)	0.050 (2)	0.0029 (17)	−0.0013 (19)	0.0088 (17)
C33	0.052 (2)	0.043 (2)	0.067 (2)	0.0033 (17)	−0.001 (2)	0.0090 (18)
C34A	0.039 (4)	0.040 (4)	0.085 (8)	−0.002 (3)	0.000 (7)	0.011 (6)
C35A	0.039 (4)	0.046 (3)	0.110 (10)	−0.005 (3)	0.006 (9)	−0.001 (7)
C36A	0.043 (3)	0.048 (3)	0.162 (16)	0.002 (2)	0.006 (10)	0.014 (8)
C34B	0.039 (4)	0.040 (4)	0.085 (8)	−0.002 (3)	0.000 (7)	0.011 (6)
C35B	0.039 (4)	0.046 (3)	0.110 (10)	−0.005 (3)	0.006 (9)	−0.001 (7)
C36B	0.043 (3)	0.048 (3)	0.162 (16)	0.002 (2)	0.006 (10)	0.014 (8)

Geometric parameters (Å, º)

Cl1—C7	1.706 (3)	N8—C19	1.366 (3)
O1—N3	1.224 (3)	N8—C26	1.467 (3)
O2—N3	1.227 (3)	N9—C21	1.480 (3)
N1—C7	1.316 (3)	N10—N11	1.340 (3)
N1—N2	1.366 (3)	N10—C28	1.346 (3)
N2—C1	1.364 (3)	N10—C29	1.463 (3)
N2—C8	1.458 (3)	N11—N12	1.317 (3)
N3—C3	1.472 (3)	N12—C27	1.361 (3)
N4—C10	1.345 (3)	C19—C20	1.391 (3)
N4—N5	1.350 (3)	C19—C24	1.404 (3)
N4—C11	1.459 (4)	C20—C21	1.373 (4)
N5—N6	1.316 (3)	C20—H20	0.94 (3)
N6—C9	1.364 (3)	C21—C22	1.404 (4)
C1—C2	1.395 (3)	C22—C23	1.368 (4)
C1—C6	1.407 (3)	C22—H22	0.96 (3)
C2—C3	1.375 (4)	C23—C24	1.397 (4)
C2—H2	0.96 (3)	C23—H23	0.92 (3)
C3—C4	1.407 (4)	C24—C25	1.419 (3)
C4—C5	1.367 (4)	C26—C27	1.485 (4)
C4—H4	0.96 (3)	C26—H26A	0.95 (3)
C5—C6	1.397 (4)	C26—H26B	0.98 (3)
C5—H5	0.94 (3)	C27—C28	1.360 (3)
C6—C7	1.419 (3)	C28—H28	0.92 (3)
C8—C9	1.486 (4)	C29—C30	1.511 (4)
C8—H8A	0.98 (3)	C29—H29A	1.00 (3)
C8—H8B	0.99 (3)	C29—H29B	1.05 (3)
C9—C10	1.359 (4)	C30—C31	1.538 (4)
C10—H10	0.93 (3)	C30—H30A	0.98 (3)
C11—C12	1.511 (4)	C30—H30B	1.05 (3)
C11—H11A	1.03 (3)	C31—C32	1.515 (5)
C11—H11B	1.00 (3)	C31—H31A	1.00 (3)
C12—C13	1.527 (4)	C31—H31B	1.07 (3)
C12—H12A	0.96 (3)	C32—C33	1.525 (5)
C12—H12B	1.00 (3)	C32—H32A	1.14 (4)
C13—C14	1.523 (4)	C32—H32B	1.03 (4)
C13—H13A	0.99 (3)	C33—C34A	1.526 (6)
C13—H13B	1.04 (3)	C33—C34B	1.526 (6)
C14—C15	1.530 (4)	C33—H33A	1.08 (4)
C14—H14A	1.04 (3)	C33—H33B	1.07 (4)
C14—H14B	1.03 (3)	C34A—C35A	1.525 (5)
C15—C16	1.523 (4)	C34A—H34A	0.9900
C15—H15A	1.07 (3)	C34A—H34B	0.9900
C15—H15B	1.01 (3)	C35A—C36A	1.516 (5)
C16—C17	1.524 (4)	C35A—H35A	0.9900
C16—H16A	1.05 (3)	C35A—H35B	0.9900
C16—H16B	1.03 (3)	C36A—H36A	0.9800

C17—C18	1.514 (4)	C36A—H36B	0.9800
C17—H17A	0.99 (3)	C36A—H36C	0.9800
C17—H17B	1.02 (3)	C34B—C35B	1.525 (5)
C18—H18A	1.06 (4)	C34B—H34C	0.9900
C18—H18B	1.01 (4)	C34B—H34D	0.9900
C18—H18C	0.99 (4)	C35B—C36B	1.516 (5)
Cl2—C25	1.709 (2)	C35B—H35C	0.9900
O3—N9	1.224 (3)	C35B—H35D	0.9900
O4—N9	1.221 (3)	C36B—H36D	0.9800
N7—C25	1.315 (3)	C36B—H36E	0.9800
N7—N8	1.369 (3)	C36B—H36F	0.9800

C7—N1—N2	105.6 (2)	N11—N12—C27	108.8 (2)
C1—N2—N1	111.3 (2)	N8—C19—C20	130.7 (2)
C1—N2—C8	127.4 (2)	N8—C19—C24	107.3 (2)
N1—N2—C8	120.4 (2)	C20—C19—C24	122.0 (2)
O1—N3—O2	123.5 (2)	C21—C20—C19	115.2 (2)
O1—N3—C3	118.0 (2)	C21—C20—H20	122.1 (15)
O2—N3—C3	118.5 (2)	C19—C20—H20	122.7 (15)
C10—N4—N5	110.6 (2)	C20—C21—C22	124.4 (2)
C10—N4—C11	129.2 (2)	C20—C21—N9	117.7 (2)
N5—N4—C11	120.2 (2)	C22—C21—N9	117.9 (2)
N6—N5—N4	107.0 (2)	C23—C22—C21	119.4 (2)
N5—N6—C9	108.8 (2)	C23—C22—H22	120.0 (17)
N2—C1—C2	130.3 (2)	C21—C22—H22	120.6 (17)
N2—C1—C6	107.2 (2)	C22—C23—C24	118.3 (3)
C2—C1—C6	122.5 (2)	C22—C23—H23	119.7 (15)
C3—C2—C1	114.6 (2)	C24—C23—H23	121.9 (15)
C3—C2—H2	121.2 (15)	C23—C24—C19	120.7 (2)
C1—C2—H2	124.2 (15)	C23—C24—C25	136.1 (2)
C2—C3—C4	124.5 (2)	C19—C24—C25	103.3 (2)
C2—C3—N3	117.5 (2)	N7—C25—C24	112.8 (2)
C4—C3—N3	118.0 (2)	N7—C25—Cl2	120.86 (18)
C5—C4—C3	119.7 (3)	C24—C25—Cl2	126.3 (2)
C5—C4—H4	122.9 (17)	N8—C26—C27	113.4 (2)
C3—C4—H4	117.3 (17)	N8—C26—H26A	106.3 (17)
C4—C5—C6	118.2 (3)	C27—C26—H26A	111.8 (17)
C4—C5—H5	120.1 (16)	N8—C26—H26B	106.6 (15)
C6—C5—H5	121.6 (16)	C27—C26—H26B	110.3 (16)
C5—C6—C1	120.4 (2)	H26A—C26—H26B	108 (2)
C5—C6—C7	136.4 (2)	C28—C27—N12	108.0 (2)
C1—C6—C7	103.2 (2)	C28—C27—C26	129.6 (2)
N1—C7—C6	112.6 (2)	N12—C27—C26	122.3 (2)
N1—C7—Cl1	120.92 (19)	N10—C28—C27	105.4 (2)
C6—C7—Cl1	126.4 (2)	N10—C28—H28	117.6 (17)
N2—C8—C9	112.6 (2)	C27—C28—H28	136.8 (17)
N2—C8—H8A	108.2 (16)	N10—C29—C30	113.2 (2)
C9—C8—H8A	110.3 (16)	N10—C29—H29A	109.1 (19)

N2—C8—H8B	107.8 (16)	C30—C29—H29A	108.5 (19)
C9—C8—H8B	113.1 (16)	N10—C29—H29B	103.5 (16)
H8A—C8—H8B	105 (2)	C30—C29—H29B	113.0 (15)
C10—C9—N6	108.3 (2)	H29A—C29—H29B	109 (2)
C10—C9—C8	130.1 (2)	C29—C30—C31	109.5 (3)
N6—C9—C8	121.6 (2)	C29—C30—H30A	110.9 (19)
N4—C10—C9	105.3 (2)	C31—C30—H30A	109.1 (19)
N4—C10—H10	122.4 (18)	C29—C30—H30B	110.5 (15)
C9—C10—H10	132.2 (18)	C31—C30—H30B	109.7 (16)
N4—C11—C12	113.2 (2)	H30A—C30—H30B	107 (2)
N4—C11—H11A	107.9 (16)	C32—C31—C30	114.5 (3)
C12—C11—H11A	107.2 (16)	C32—C31—H31A	110 (2)
N4—C11—H11B	109.0 (15)	C30—C31—H31A	108 (2)
C12—C11—H11B	109.6 (15)	C32—C31—H31B	107.6 (18)
H11A—C11—H11B	110 (2)	C30—C31—H31B	109.0 (17)
C11—C12—C13	110.7 (3)	H31A—C31—H31B	108 (3)
C11—C12—H12A	109.3 (18)	C31—C32—C33	113.8 (3)
C13—C12—H12A	110.7 (18)	C31—C32—H32A	108.2 (18)
C11—C12—H12B	108.0 (16)	C33—C32—H32A	110.7 (18)
C13—C12—H12B	111.0 (16)	C31—C32—H32B	110 (2)
H12A—C12—H12B	107 (2)	C33—C32—H32B	108 (2)
C14—C13—C12	114.8 (3)	H32A—C32—H32B	106 (3)
C14—C13—H13A	110.2 (17)	C32—C33—C34A	120.2 (9)
C12—C13—H13A	105.5 (17)	C32—C33—C34B	106.2 (10)
C14—C13—H13B	109.4 (16)	C32—C33—H33A	108.2 (18)
C12—C13—H13B	109.6 (16)	C34A—C33—H33A	107 (2)
H13A—C13—H13B	107 (2)	C34B—C33—H33A	115 (2)
C13—C14—C15	113.4 (3)	C32—C33—H33B	111 (2)
C13—C14—H14A	109.8 (17)	C34A—C33—H33B	108 (2)
C15—C14—H14A	106.1 (17)	C34B—C33—H33B	115 (3)
C13—C14—H14B	109.1 (17)	H33A—C33—H33B	102 (3)
C15—C14—H14B	110.3 (17)	C35A—C34A—C33	116.1 (12)
H14A—C14—H14B	108 (2)	C35A—C34A—H34A	108.3
C16—C15—C14	113.4 (3)	C33—C34A—H34A	108.3
C16—C15—H15A	111.2 (16)	C35A—C34A—H34B	108.3
C14—C15—H15A	107.7 (16)	C33—C34A—H34B	108.3
C16—C15—H15B	109.6 (18)	H34A—C34A—H34B	107.4
C14—C15—H15B	109.5 (18)	C36A—C35A—C34A	113.4 (5)
H15A—C15—H15B	105 (2)	C36A—C35A—H35A	108.9
C15—C16—C17	112.8 (3)	C34A—C35A—H35A	108.9
C15—C16—H16A	108.3 (15)	C36A—C35A—H35B	108.9
C17—C16—H16A	110.2 (14)	C34A—C35A—H35B	108.9
C15—C16—H16B	111.9 (17)	H35A—C35A—H35B	107.7
C17—C16—H16B	108.5 (17)	C35A—C36A—H36A	109.5
H16A—C16—H16B	105 (2)	C35A—C36A—H36B	109.5
C18—C17—C16	113.3 (3)	H36A—C36A—H36B	109.5
C18—C17—H17A	111.5 (17)	C35A—C36A—H36C	109.5
C16—C17—H17A	107.5 (17)	H36A—C36A—H36C	109.5

C18—C17—H17B	109.4 (18)	H36B—C36A—H36C	109.5
C16—C17—H17B	110.7 (17)	C35B—C34B—C33	110.8 (14)
H17A—C17—H17B	104 (2)	C35B—C34B—H34C	109.5
C17—C18—H18A	113 (2)	C33—C34B—H34C	109.5
C17—C18—H18B	112 (2)	C35B—C34B—H34D	109.5
H18A—C18—H18B	102 (3)	C33—C34B—H34D	109.5
C17—C18—H18C	113 (3)	H34C—C34B—H34D	108.1
H18A—C18—H18C	108 (3)	C36B—C35B—C34B	113.3 (5)
H18B—C18—H18C	108 (3)	C36B—C35B—H35C	108.9
C25—N7—N8	105.47 (19)	C34B—C35B—H35C	108.9
C19—N8—N7	111.2 (2)	C36B—C35B—H35D	108.9
C19—N8—C26	128.1 (2)	C34B—C35B—H35D	108.9
N7—N8—C26	120.7 (2)	H35C—C35B—H35D	107.7
O4—N9—O3	123.7 (2)	C35B—C36B—H36D	109.5
O4—N9—C21	118.4 (2)	C35B—C36B—H36E	109.5
O3—N9—C21	117.9 (2)	H36D—C36B—H36E	109.5
N11—N10—C28	110.5 (2)	C35B—C36B—H36F	109.5
N11—N10—C29	120.7 (2)	H36D—C36B—H36F	109.5
C28—N10—C29	128.7 (2)	H36E—C36B—H36F	109.5
N12—N11—N10	107.2 (2)		

C7—N1—N2—C1	−1.0 (3)	C28—N10—N11—N12	−0.2 (3)
C7—N1—N2—C8	−171.4 (2)	C29—N10—N11—N12	178.9 (2)
C10—N4—N5—N6	−0.2 (3)	N10—N11—N12—C27	−0.1 (3)
C11—N4—N5—N6	179.7 (2)	N7—N8—C19—C20	179.6 (2)
N4—N5—N6—C9	0.0 (3)	C26—N8—C19—C20	−3.2 (4)
N1—N2—C1—C2	−178.6 (2)	N7—N8—C19—C24	−0.2 (3)
C8—N2—C1—C2	−9.0 (4)	C26—N8—C19—C24	177.1 (2)
N1—N2—C1—C6	0.5 (3)	N8—C19—C20—C21	179.3 (2)
C8—N2—C1—C6	170.1 (2)	C24—C19—C20—C21	−1.0 (4)
N2—C1—C2—C3	179.2 (3)	C19—C20—C21—C22	0.6 (4)
C6—C1—C2—C3	0.2 (4)	C19—C20—C21—N9	179.7 (2)
C1—C2—C3—C4	0.5 (4)	O4—N9—C21—C20	5.6 (3)
C1—C2—C3—N3	−178.6 (2)	O3—N9—C21—C20	−174.5 (2)
O1—N3—C3—C2	178.4 (2)	O4—N9—C21—C22	−175.3 (2)
O2—N3—C3—C2	−0.9 (3)	O3—N9—C21—C22	4.6 (4)
O1—N3—C3—C4	−0.7 (3)	C20—C21—C22—C23	0.2 (4)
O2—N3—C3—C4	−180.0 (2)	N9—C21—C22—C23	−178.9 (2)
C2—C3—C4—C5	−0.6 (4)	C21—C22—C23—C24	−0.6 (4)
N3—C3—C4—C5	178.4 (2)	C22—C23—C24—C19	0.3 (4)
C3—C4—C5—C6	0.0 (4)	C22—C23—C24—C25	180.0 (3)
C4—C5—C6—C1	0.7 (4)	N8—C19—C24—C23	−179.6 (2)
C4—C5—C6—C7	−179.6 (3)	C20—C19—C24—C23	0.6 (4)
N2—C1—C6—C5	180.0 (2)	N8—C19—C24—C25	0.6 (3)
C2—C1—C6—C5	−0.9 (4)	C20—C19—C24—C25	−179.2 (2)
N2—C1—C6—C7	0.2 (3)	N8—N7—C25—C24	0.7 (3)
C2—C1—C6—C7	179.4 (2)	N8—N7—C25—Cl2	−179.31 (17)
N2—N1—C7—C6	1.2 (3)	C23—C24—C25—N7	179.4 (3)

N2—N1—C7—Cl1	−179.25 (18)	C19—C24—C25—N7	−0.8 (3)
C5—C6—C7—N1	179.4 (3)	C23—C24—C25—Cl2	−0.5 (5)
C1—C6—C7—N1	−0.9 (3)	C19—C24—C25—Cl2	179.23 (19)
C5—C6—C7—Cl1	−0.1 (5)	C19—N8—C26—C27	−77.4 (3)
C1—C6—C7—Cl1	179.6 (2)	N7—N8—C26—C27	99.6 (3)
C1—N2—C8—C9	−73.4 (3)	N11—N12—C27—C28	0.3 (3)
N1—N2—C8—C9	95.3 (3)	N11—N12—C27—C26	−177.2 (2)
N5—N6—C9—C10	0.2 (3)	N8—C26—C27—C28	111.7 (3)
N5—N6—C9—C8	−179.2 (2)	N8—C26—C27—N12	−71.4 (3)
N2—C8—C9—C10	106.5 (3)	N11—N10—C28—C27	0.3 (3)
N2—C8—C9—N6	−74.2 (3)	C29—N10—C28—C27	−178.6 (2)
N5—N4—C10—C9	0.3 (3)	N12—C27—C28—N10	−0.4 (3)
C11—N4—C10—C9	−179.5 (3)	C26—C27—C28—N10	176.8 (2)
N6—C9—C10—N4	−0.3 (3)	N11—N10—C29—C30	95.7 (3)
C8—C9—C10—N4	179.1 (3)	C28—N10—C29—C30	−85.4 (3)
C10—N4—C11—C12	−109.4 (3)	N10—C29—C30—C31	176.9 (3)
N5—N4—C11—C12	70.8 (3)	C29—C30—C31—C32	173.6 (3)
N4—C11—C12—C13	−178.0 (2)	C30—C31—C32—C33	−63.7 (4)
C11—C12—C13—C14	178.8 (2)	C31—C32—C33—C34A	−159 (2)
C12—C13—C14—C15	−54.8 (4)	C31—C32—C33—C34B	−160.8 (19)
C13—C14—C15—C16	−165.4 (3)	C32—C33—C34A—C35A	−178 (2)
C14—C15—C16—C17	−175.9 (3)	C33—C34A—C35A—C36A	−174 (2)
C15—C16—C17—C18	−176.2 (3)	C32—C33—C34B—C35B	177 (3)
C25—N7—N8—C19	−0.3 (3)	C33—C34B—C35B—C36B	−178 (3)
C25—N7—N8—C26	−177.8 (2)		

Hydrogen-bond geometry (Å, º)

*Cg*1, Cg2 and *Cg*3 are the centroids of the N7/N8/C19/C24/C25, N10/N11/N12/C27/C28 and C19–C24 rings, respectively

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8*A*···O2^{i}	0.98 (3)	2.62 (3)	3.348 (3)	132 (2)
C10—H10···N6^{ii}	0.93 (3)	2.57 (3)	3.377 (3)	145 (2)
C26—H26*A*···O4^{iii}	0.95 (3)	2.54 (3)	3.240 (3)	131 (2)
C26—H26*B*···Cl2^{iv}	0.98 (3)	2.82 (3)	3.682 (3)	147 (2)
C28—H28···N12^{iv}	0.92 (3)	2.45 (3)	3.298 (3)	152 (2)
C29—H29*B*···N11^{iv}	1.05 (3)	2.63 (3)	3.594 (4)	153 (2)
C29—H29*B*···N12^{iv}	1.05 (3)	2.65 (3)	3.476 (3)	135 (2)

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