Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

Ring-strain release in neutral and dicationic 7,8,17,18-tetrabromo-5,10,15,20-tetraphenylporphyrin: crystal structures of $C_{44}H_{26}Br_4N_4$ and $C_{44}H_{28}Br_4N_4^{2+}\cdot 2ClO_4^-\cdot 3CH_2Cl_2$

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Received 22 April 2016
Accepted 2 May 2016

Edited by W. T. A. Harrison, University of Aberdeen, Scotland

Keywords: crystal structure; prophyrin; hydrogen bonding; ring puckering.

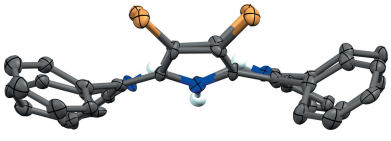
CCDC references: 1477658; 1477657

Supporting information: this article has supporting information at journals.iucr.org/e

Two porphyrin complexes were studied to determine the effects of protonation on ring deformation within the porphyrin. The porphyrin 7,8,17,18-tetrabromo-5,10,15,20-tetraphenylporphyrin, $C_{44}H_{26}Br_4N_4$, was selected because the neutral species is readily doubly protonated to yield a dication, which was crystallized here with perchlorate counter-ions as a dichloromethane trisolvate, $C_{44}H_{28}Br_4N_4^{2+}\cdot 2ClO_4^-\cdot 3CH_2Cl_2$. The centrosymmetric neutral species is observed to have a mild 'ruffling' of the pyrrole rings and is essentially planar throughout; intramolecular N—H···N hydrogen bonds occur. In contrast, the dication exhibits considerable deformation, with the pyrrole rings oriented well out of the plane of the porphyrin, resulting in a 'saddle' conformation of the ring. The charged species forms N—H···O hydrogen bonds to the perchlorate anions, which lie above and below the plane of the porphyrin ring. Distortions to the planarity of the pyrrole rings in both cases are very minor. The characterization of the neutral species represents a low-temperature redetermination of the previous room-temperature analyses [Zou *et al.* (1995). *Acta Cryst.* C**51**, 760–761; Rayati *et al.* (2008). *Polyhedron*, pp. 2285–2290], which showed disorder and physically unrealistic displacement parameters.

1. Chemical context

Ring folding in porphyrins has long been of interest with characteristics such as ruffling, doming and saddling resulting in strain relief about the ring. In particular, the interactions within the constrained environment of the tetra-pyrrole core predominantly affect the orientation of the pyrrole rings. Two porphyrin molecules were studied to examine the effects of protonation of the pyrrole nitrogen atoms upon the overall geometry of the porphyrin ring systems. The porphyrin: 7,8,17,18-tetrabromo-5,10,15,20-tetraphenylporphyrin (I), H_2TPPBr_4 was adopted for this study. It readily accepts two protons forming a dicationic species (II), $[H_4TPPBr_4]^{2+}$. The neutral porphyrin (I) has previously been reported in two different, room-temperature determinations (Zou *et al.*, 1995; Rayati *et al.*, 2008). However, those two structures display disorder that is not present in the low-temperature determination provided herein.



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2. Structural commentary

The neutral porphyrin (I) was found to crystallize about the center of symmetry at the origin (Fig. 1). Distinctly different, the dicationic porphyrin (II) was found to crystallize with one

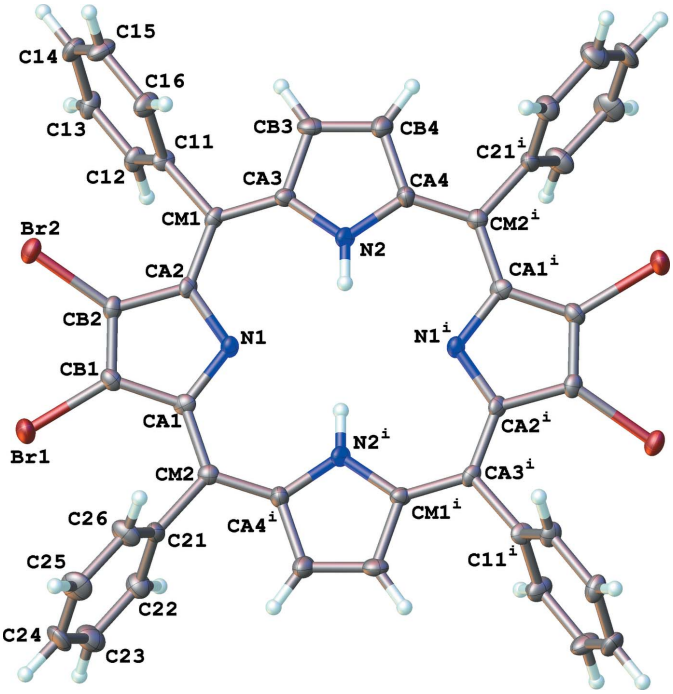


Figure 1
Structure and labeling scheme of (I). Atomic displacement parameters are depicted at 50% probability. H atoms are depicted as spheres of an arbitrary radius. [Symmetry code: (i) $-x$, $-y$, $-z$.]

complete porphyrin dication, two perchlorate ions and three molecules of dichloromethane solvent of crystallization in the asymmetric unit (Fig. 2). Thus, the geometry of (I) is influenced by symmetry, while the geometry of (II) is independent

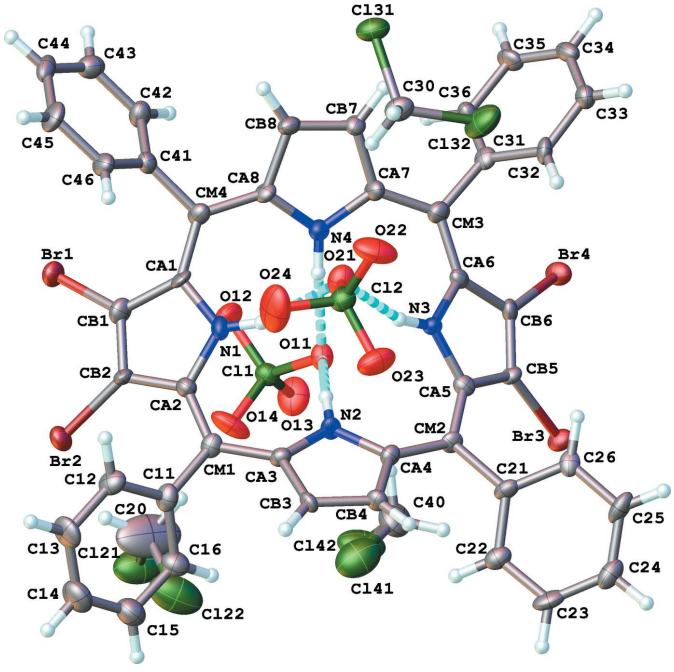


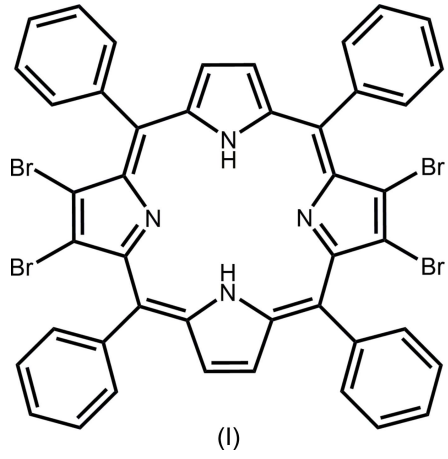
Figure 2
Structure and labelling scheme of (II). Atomic displacement parameters are depicted at 50% probability. H atoms are depicted as spheres of an arbitrary radius. Hydrogen bonds are represented as light-blue dashed lines.

Table 1
Pyrrole periplanar angles (°).

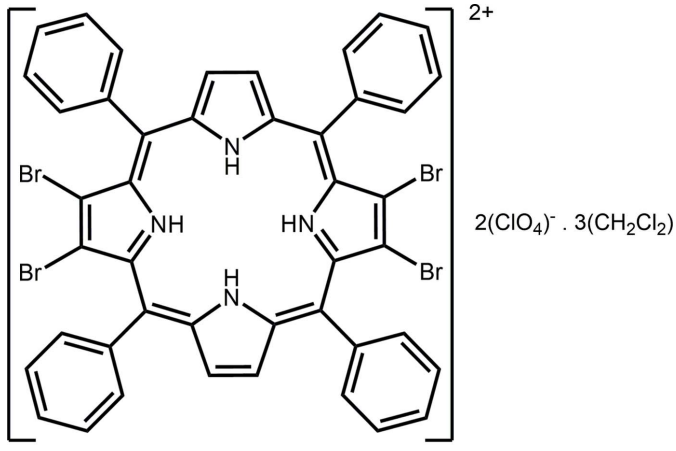
Angles with respect to the mean four atom *meta*-carbon plane. A 'negative' angle represents an arbitrary orientation with the pyrrole N atom below the mean porphyrin plane.

Pyrrole Ring	(I)	(II)
N1—*CA*1—*CB*1—*CB*2—*CA*2	3.0 (3)	31.0 (5)
N2—*CA*3—*CB*3—*CB*4—*CA*4	6.5 (3)	−30.1 (5)
N3—*CA*5—*CB*5—*CB*6—*CA*6		33.6 (4)
N4—*CA*7—*CB*7—*CB*8—*CA*8		−23.2 (3)

of such constraints. In both studies, we elected to use the *meta*-carbon atoms of the porphyrin ring (labeled as CM*n* in the Figures; *n* = atom number) as the basis for an arbitrary mean plane for analyzing distortions.



(I)



(II)

The neutral compound (I) exhibits very mild 'ruffling' of the pyrrole rings. The two independent pyrrole rings form periplanar angles of 3.0 (3) and 6.5 (3)° with the four porphyrin *meta*-carbon atoms (Table 1). This is largely influenced by the lack of steric hindrance of the two hydrogen atoms within the core of the porphyrin ring (Fig. 3). This lack of hindrance is also reflected in the intramolecular N—H···N hydrogen bonds formed in the core that have typical *D*···*A* distances

Table 2
Hydrogen-bond geometry (Å, °) for (I).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···N1	0.88	2.47	2.973 (5)	117
N2—H2···N1^{i}	0.88	2.40	2.921 (5)	118

Symmetry code: (i) $-x, -y, -z$.

Table 3
Deviations from pyrrole planes for (I) and (II) (Å).

Atom	(I)	(II)
N1	−0.008 (3)	−0.012 (7)
*CA*1	−0.004 (3)	0.006 (7)
*CA*2	0.015 (3)	0.013 (7)
*CB*1	0.014 (3)	0.002 (7)
*CB*2	−0.018 (3)	−0.009 (7)
Br1	−0.117 (8)	−0.28 (2)
Br2	0.403 (7)	−0.28 (2)
N2	0.006 (3)	0.021 (7)
*CA*3	−0.001 (3)	−0.006 (7)
*CA*4	−0.009 (3)	−0.027 (7)
*CB*3	−0.005 (3)	−0.011 (7)
*CB*4	0.008 (3)	0.023 (7)
N3		−0.015 (6)
*CA*5		0.017 (6)
*CA*6		0.007 (7)
*CB*5		−0.013 (7)
*CB*6		0.004 (7)
Br3		−0.283 (18)
Br4		−0.114 (19)
N4		0.005 (8)
*CA*7		0.000 (7)
*CA*8		−0.007 (8)
*CB*7		−0.004 (8)
*CB*8		0.006 (8)

(Table 2). However, these intramolecular hydrogen bonds are not well directed, as demonstrated by the relatively constrained N—H···N angles. The pyrrole rings experience very little distortion, with the greatest deviation from the mean-plane being −0.018 (3) Å for *CB*2 (Table 3). The ruffling of the ring is reflected more so in the deviations of the bromine and *ipso*-carbon atoms of the phenyl groups from the mean plane (Table 4). It should be noted that due to the center of symmetry, the transannular pairs of pyrrole rings are tilted in opposite directions with respect to the mean plane. Presumably this also plays a role in reducing steric hindrance of the pyrrole hydrogen atoms.

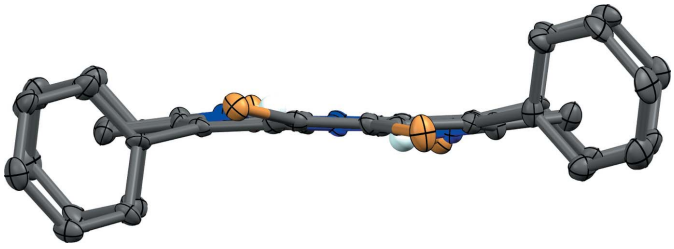


Figure 3
View through the porphyrin plane of (I) showing ring 'ruffling'. H atoms, except pyrrole H atoms, have been omitted for clarity.

Table 4
Deviations of peripheral atoms from mean *meta*-carbon plane for (I) and (II) (Å).

Atom	(I)	(II)
C11	−0.240 (7)	−0.038 (19)
C21	0.205 (8)	0.194 (18)
C31		0.061 (18)
C41		0.232 (19)

Table 5
Hydrogen-bond geometry (Å, °) for (II).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N2	0.88	2.57	3.018 (12)	113
N1—H1···O21	0.88	2.12	2.956 (14)	158
N2—H2···N1	0.88	2.60	3.018 (12)	110
N2—H2···N3	0.88	2.59	3.026 (12)	111
N2—H2···O11	0.88	2.07	2.896 (12)	157
N3—H3···O21	0.88	2.08	2.932 (13)	162
N4—H4···N3	0.88	2.62	3.034 (12)	110
N4—H4···O11	0.88	2.01	2.844 (13)	159

In contrast the dicationic porphyrin (II) relieves strain by adopting a 'saddled' conformation (Fig. 4). In this fashion, steric repulsion between the four hydrogen atoms intruding on the core of the porphyrin is significantly reduced. Furthermore, due to the presence of charge-balancing perchlorate anions, each pair of transannular pyrrole nitrogen atoms form hydrogen bonds to one oxygen atom of either perchlorate anion (N1/N3···O21, N2/N4···O25, Fig. 2, Table 5).

Surprisingly, the pyrrole rings in (II) do not adopt any crystallographic symmetry. Crystallographically, each pair of rings oriented 'up' and 'down' (arbitrarily defined) form different angles with respect to the *meta*-carbon plane. Inspection of the structure shows that the bromo-pyrrole rings are inclined in the same fashion (we have arbitrarily defined this as 'down' or a negative periplanar angle with regards to the pyrrole nitrogen atoms with respect to the porphyrin mean plane). In contrast with (I), the pyrrole rings in (II) form angles ±30° with respect to the mean porphyrin plane (Table 1). Compared with (I) wherein one bromine atom is deformed 'above' the pyrrole plane and the other 'below', the bromine atoms in (II) are all oriented out of the mean plane of their respective pyrrole rings in the same fashion (*i.e.* all of the deviations from the mean pyrrole plane are negative). The atoms of the pyrrole rings are essentially co-planar with the largest deviation from the mean plane for any pyrrole atom being −0.027 (7) Å for *CA*4 (Table 3).

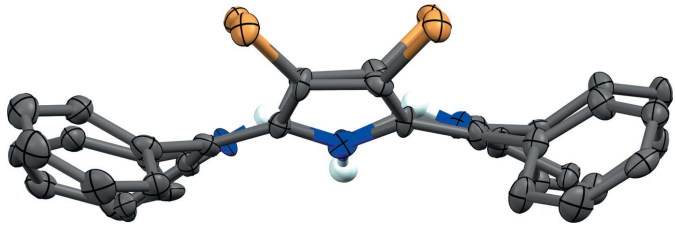


Figure 4
View through the porphyrin plane of (II) demonstrating ring 'saddling'. H atoms, except pyrrole H atoms, have been omitted for clarity.

Table 6
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	$C_{44}H_{26}Br_4N_4$	$C_{44}H_{28}Br_4N_4^{2+}\cdot 2ClO_4^-\cdot 3CH_2Cl_2$
M_r	930.33	1386.02
Crystal system, space group	Monoclinic, $P2_1/n$	Monoclinic, Pn
Temperature (K)	130	130
a, b, c (Å)	13.883 (3), 6.7448 (13), 19.110 (4)	12.903 (3), 13.761 (3), 14.876 (3)
β (°)	102.00 (3)	96.67 (3)
V (Å^3)	1750.3 (7)	2623.5 (10)
Z	2	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	4.64	3.53
Crystal size (mm)	0.15 × 0.10 × 0.05	0.33 × 0.17 × 0.06
Data collection		
Diffractometer	Enraf–Nonius fast area-detector	Enraf–Nonius fast area-detector
Absorption correction	Part of the refinement model (ΔF) (*DIFABS*; Walker & Stuart, 1983)	Part of the refinement model (ΔF) (*DIFABS*; Walker & Stuart, 1983)
T_{min}, T_{max}	0.72, 1.00	0.65, 1.00
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	4589, 4589, 3439	11251, 11251, 8745
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.701	0.703
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.059, 0.156, 1.08	0.060, 0.185, 1.06
No. of reflections	4589	11251
No. of parameters	235	640
No. of restraints	0	2
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.17, −1.41	1.03, −1.05
Absolute structure	–	Classical Flack method preferred over Parsons because s.u. lower (Flack, 1983)
Absolute structure parameter	–	−0.032 (14)

Computer programs: *MADNES* (Pflugrath & Messerschmidt, 1989), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *OLEX2* (Dolomanov *et al.*, 2009), *Mercury* (Macrae *et al.*, 2008) and *publCIF* (Westrip, 2010).

Comparing bond distances around the neutral and dicationic porphyrin ring systems reveals little change in the bond distances associated with the pyrrole rings or backbone (see CIF files). Thus, in either a neutral or charged state the porphyrin consists largely of delocalized bonds, rather than the single-bond/double-bond formalism.

3. Supramolecular features

The neutral compound (I) packs with typical van der Waals contacts. Potential close contacts from C16 to the pyrrole of an adjacent molecule have the shortest heavy-atom contact around 3.45 Å.

In contrast, compound (II) is formed with hydrogen bonds from the pyrrole nitrogen atoms to perchlorate oxygen atoms (Fig. 2, Table 5 for details). Remaining intermolecular contacts throughout the structure are all usual van der Waals interactions.

4. Database survey

Inspection of the Cambridge Structure Database (Version 5.38 plus 1 update; Groom *et al.*, 2016) reveals three structures that incorporate the H_2TPPBr_4 moiety. Two structures (GOGNIA: Rayati *et al.*, 2008; LINPON: Zou *et al.*, 1995) are room-temperature determinations of the low-temperature structure (I) reported herein. Examination of those two structures reveals several underlying problems, such as disorder and unreasonable atomic displacement parameters that are not present in this study. The third compound that incorporates H_2TPPBr_4 is a co-crystallant with C60 fullerene (TUBPAJ: Karunanithi & Bhyrappa, 2015). To the best of our knowledge, the dicationic species (II) has not been structurally characterized in any form.

5. Synthesis and crystallization

Compound (I) was prepared following literature procedures (Callot, 1973; Crossley *et al.*, 1991). Compound (II) was prepared with procedures as previously described (Cheng *et al.*, 1997).

6. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 6. All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. C-bound hydrogen atoms were included in geometrically calculated positions. N-bound hydrogen atoms were initially located from a difference Fourier map and subsequently

included using a riding model. U_{iso}(H) = 1.2U_{eq}(C/N); C—H distances were set at 0.95 Å and N—H set at 0.88 Å for (I) and (II). Due to the age of the data and an infelicity in data archiving, only the printed structure-factor tables and final residuals file were available. Data were reconstituted from these tables into an *h k l F* $\sigma(F)$ format file and the atomic models refined against these to result in the structures contained herein. It was not considered reasonable to attempt to resynthesize and recrystallize the compounds and collect new intensity data.

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supporting information

Acta Cryst. (2016). E**72**, 824-828 [https://doi.org/10.1107/S2056989016007349]

Ring-strain release in neutral and dicationic 7,8,17,18-tetrabromo-5,10,15,20-tetraphenylporphyrin: crystal structures of $C_{44}H_{26}Br_4N_4$ and $C_{44}H_{28}Br_4N_4^{2+}\cdot 2ClO_4^-\cdot 3CH_2Cl_2$

W. Robert Scheidt, Hugues F. Duval and Allen G. Oliver

Computing details

For both compounds, data collection: *MADNES* (Pflugrath & Messerschmidt, 1989); cell refinement: *MADNES* (Pflugrath & Messerschmidt, 1989); data reduction: *MADNES* (Pflugrath & Messerschmidt, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *publCIF* (Westrip, 2010).

(I) 7,8,17,18-Tetrabromo-5,10,15,20-tetraphenylporphyrin

Crystal data

$C_{44}H_{26}Br_4N_4$
M_r = 930.33
Monoclinic, $P2_1/n$
a = 13.883 (3) Å
b = 6.7448 (13) Å
c = 19.110 (4) Å
β = 102.00 (3)°
V = 1750.3 (7) Å^3
Z = 2
$F(000)$ = 916
D_x = 1.765 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 250 reflections
θ = 2.5–20.5°
μ = 4.64 mm^{-1}
T = 130 K
Prism, dark blue
0.15 × 0.10 × 0.05 mm

Data collection

Enraf–Nonius fast area-detector diffractometer
Radiation source: ROTATING ANODE
Graphite monochromator
Detector resolution: 8.53 pixels mm^{-1}
ELLIPSOID–MASK FITTING scans
Absorption correction: part of the refinement model (ΔF)
(DIFABS; Walker & Stuart, 1983)
T_{min} = 0.72, T_{max} = 1.00
4589 measured reflections
4589 independent reflections
3439 reflections with $I > 2\sigma(I)$
θ_{max} = 29.9°, θ_{min} = 3.0°
h = −19→18
k = 0→9
l = 0→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.156
S = 1.08
4589 reflections
235 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map	$w = 1/[\sigma^2(F_o^2) + (0.0649P)^2 + 9.9345P]$ where $P = (F_o^2 + 2F_c^2)/3$
Hydrogen site location: inferred from neighbouring sites	$(\Delta/\sigma)_{max} < 0.001$
H-atom parameters constrained	$\Delta\rho_{max} = 1.17$ e Å^{-3}
	$\Delta\rho_{min} = -1.41$ e Å^{-3}

Special details

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.1162 (3)	0.2085 (6)	0.02369 (19)	0.0155 (7)
N2	−0.0795 (3)	0.1542 (6)	0.0612 (2)	0.0176 (7)
H2	−0.0527	0.1021	0.0276	0.021*
CA1	0.2010 (3)	0.2138 (6)	−0.0031 (2)	0.0163 (8)
CA2	0.1182 (3)	0.3683 (6)	0.0676 (2)	0.0148 (8)
CA3	−0.0411 (3)	0.3106 (7)	0.1040 (2)	0.0156 (8)
CA4	−0.1664 (3)	0.0898 (7)	0.0785 (2)	0.0183 (8)
CB1	0.2583 (3)	0.3860 (7)	0.0253 (2)	0.0178 (8)
CB2	0.2072 (3)	0.4848 (7)	0.0667 (2)	0.0172 (8)
CB3	−0.1091 (3)	0.3476 (7)	0.1503 (3)	0.0204 (9)
HB3	−0.1024	0.4471	0.1862	0.025*
CB4	−0.1835 (3)	0.2172 (7)	0.1340 (3)	0.0223 (9)
HB4	−0.2389	0.2110	0.1560	0.027*
CM1	0.0469 (3)	0.4092 (6)	0.1078 (2)	0.0151 (8)
CM2	0.2222 (3)	0.0767 (6)	−0.0529 (2)	0.0161 (8)
C11	0.0682 (3)	0.5628 (7)	0.1657 (2)	0.0161 (8)
C12	0.1363 (3)	0.5217 (7)	0.2295 (2)	0.0198 (9)
H12	0.1702	0.3985	0.2345	0.024*
C13	0.1550 (4)	0.6569 (7)	0.2854 (3)	0.0218 (9)
H13	0.2013	0.6278	0.3283	0.026*
C14	0.1035 (4)	0.8386 (8)	0.2771 (3)	0.0258 (10)
H14	0.1149	0.9329	0.3148	0.031*
C15	0.0370 (4)	0.8803 (8)	0.2150 (3)	0.0265 (10)
H15	0.0033	1.0037	0.2101	0.032*
C16	0.0185 (4)	0.7440 (7)	0.1589 (3)	0.0244 (10)
H16	−0.0279	0.7743	0.1163	0.029*
C21	0.3085 (3)	0.1125 (7)	−0.0877 (3)	0.0202 (9)
C22	0.3923 (4)	−0.0027 (8)	−0.0723 (3)	0.0242 (10)
H22	0.3978	−0.1064	−0.0380	0.029*
C23	0.4683 (4)	0.0344 (9)	−0.1075 (3)	0.0330 (12)
H23	0.5257	−0.0462	−0.0973	0.040*
C24	0.4629 (4)	0.1832 (9)	−0.1563 (3)	0.0299 (11)
H24	0.5167	0.2083	−0.1787	0.036*
C25	0.3791 (4)	0.2968 (9)	−0.1728 (3)	0.0309 (11)

H25	0.3749	0.4005	−0.2069	0.037*
C26	0.3000 (4)	0.2606 (8)	−0.1398 (3)	0.0261 (10)
H26	0.2411	0.3357	−0.1526	0.031*
Br2	0.24434 (4)	0.73342 (7)	0.10682 (2)	0.02175 (14)
Br1	0.38509 (4)	0.46336 (8)	0.01738 (3)	0.02782 (16)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0159 (17)	0.0179 (18)	0.0124 (16)	−0.0043 (14)	0.0023 (13)	−0.0017 (13)
N2	0.0131 (16)	0.0218 (19)	0.0163 (16)	−0.0018 (14)	−0.0005 (14)	−0.0062 (14)
CA1	0.021 (2)	0.0157 (19)	0.0128 (18)	0.0005 (16)	0.0049 (16)	0.0029 (15)
CA2	0.0117 (18)	0.0167 (19)	0.0135 (17)	−0.0008 (14)	−0.0031 (15)	−0.0017 (15)
CA3	0.0146 (19)	0.019 (2)	0.0132 (18)	0.0013 (15)	0.0018 (15)	−0.0031 (15)
CA4	0.0163 (19)	0.020 (2)	0.019 (2)	−0.0044 (16)	0.0054 (17)	−0.0036 (17)
CB1	0.0152 (19)	0.023 (2)	0.0158 (19)	−0.0011 (16)	0.0039 (15)	0.0018 (16)
CB2	0.017 (2)	0.018 (2)	0.0145 (19)	−0.0030 (16)	−0.0015 (16)	0.0002 (16)
CB3	0.020 (2)	0.022 (2)	0.021 (2)	0.0066 (17)	0.0058 (18)	−0.0029 (17)
CB4	0.017 (2)	0.023 (2)	0.026 (2)	−0.0001 (17)	0.0023 (18)	−0.0072 (18)
CM1	0.0182 (19)	0.0144 (19)	0.0106 (18)	−0.0013 (15)	−0.0019 (15)	−0.0013 (14)
CM2	0.0170 (19)	0.017 (2)	0.0146 (18)	0.0008 (15)	0.0030 (16)	0.0007 (15)
C11	0.0137 (18)	0.020 (2)	0.0120 (18)	0.0034 (15)	−0.0036 (15)	0.0001 (15)
C12	0.023 (2)	0.023 (2)	0.0120 (18)	−0.0046 (17)	−0.0002 (17)	−0.0020 (16)
C13	0.025 (2)	0.020 (2)	0.018 (2)	−0.0052 (17)	−0.0025 (18)	−0.0005 (17)
C14	0.029 (2)	0.025 (2)	0.023 (2)	−0.007 (2)	0.005 (2)	−0.0124 (19)
C15	0.027 (2)	0.022 (2)	0.028 (2)	0.0071 (19)	0.000 (2)	−0.009 (2)
C16	0.021 (2)	0.026 (2)	0.022 (2)	0.0019 (18)	−0.0048 (18)	−0.0073 (18)
C21	0.0147 (19)	0.024 (2)	0.023 (2)	−0.0047 (17)	0.0060 (17)	−0.0086 (18)
C22	0.021 (2)	0.026 (2)	0.026 (2)	0.0004 (18)	0.0040 (19)	0.0017 (19)
C23	0.020 (2)	0.044 (3)	0.035 (3)	0.002 (2)	0.006 (2)	−0.003 (2)
C24	0.021 (2)	0.042 (3)	0.032 (3)	−0.009 (2)	0.017 (2)	−0.004 (2)
C25	0.038 (3)	0.038 (3)	0.020 (2)	−0.002 (2)	0.014 (2)	0.007 (2)
C26	0.023 (2)	0.035 (3)	0.022 (2)	0.002 (2)	0.0089 (19)	0.008 (2)
Br2	0.0263 (3)	0.0177 (2)	0.0210 (2)	−0.00664 (17)	0.00424 (18)	−0.00363 (16)
Br1	0.0226 (3)	0.0307 (3)	0.0331 (3)	−0.01189 (19)	0.0126 (2)	−0.0098 (2)

Geometric parameters (Å, º)

N1—CA2	1.363 (5)	C11—C16	1.396 (6)
N1—CA1	1.378 (6)	C11—C12	1.407 (6)
N2—CA3	1.372 (6)	C12—C13	1.387 (6)
N2—CA4	1.385 (5)	C12—H12	0.9500
N2—H2	0.8800	C13—C14	1.411 (7)
CA1—CM2	1.402 (6)	C13—H13	0.9500
CA1—CB1	1.447 (6)	C14—C15	1.372 (7)
CA2—CM1	1.400 (6)	C14—H14	0.9500
CA2—CB2	1.467 (6)	C15—C16	1.395 (7)
CA3—CM1	1.380 (6)	C15—H15	0.9500

CA3—CB3	1.444 (6)	C16—H16	0.9500
CA4—CM2^{i}	1.395 (6)	C21—C22	1.378 (7)
CA4—CB4	1.422 (6)	C21—C26	1.398 (7)
CB1—CB2	1.344 (6)	C22—C23	1.387 (7)
CB1—Br1	1.872 (4)	C22—H22	0.9500
CB2—Br2	1.871 (4)	C23—C24	1.361 (8)
CB3—CB4	1.344 (7)	C23—H23	0.9500
CB3—HB3	0.9500	C24—C25	1.375 (8)
CB4—HB4	0.9500	C24—H24	0.9500
CM1—C11	1.500 (6)	C25—C26	1.397 (7)
CM2—CA4^{i}	1.395 (6)	C25—H25	0.9500
CM2—C21	1.505 (6)	C26—H26	0.9500

CA2—N1—CA1	107.4 (3)	C16—C11—CM1	121.2 (4)
CA3—N2—CA4	110.4 (4)	C12—C11—CM1	119.8 (4)
CA3—N2—H2	124.8	C13—C12—C11	121.5 (5)
CA4—N2—H2	124.8	C13—C12—H12	119.2
N1—CA1—CM2	123.5 (4)	C11—C12—H12	119.2
N1—CA1—CB1	109.1 (4)	C12—C13—C14	118.3 (4)
CM2—CA1—CB1	127.4 (4)	C12—C13—H13	120.8
N1—CA2—CM1	124.5 (4)	C14—C13—H13	120.8
N1—CA2—CB2	109.0 (4)	C15—C14—C13	120.6 (4)
CM1—CA2—CB2	126.5 (4)	C15—C14—H14	119.7
N2—CA3—CM1	129.2 (4)	C13—C14—H14	119.7
N2—CA3—CB3	106.0 (4)	C14—C15—C16	120.9 (5)
CM1—CA3—CB3	124.7 (4)	C14—C15—H15	119.6
N2—CA4—CM2^{i}	128.1 (4)	C16—C15—H15	119.6
N2—CA4—CB4	106.2 (4)	C15—C16—C11	119.8 (4)
CM2^{i}—CA4—CB4	125.5 (4)	C15—C16—H16	120.1
CB2—CB1—CA1	107.6 (4)	C11—C16—H16	120.1
CB2—CB1—Br1	121.9 (4)	C22—C21—C26	119.8 (4)
CA1—CB1—Br1	130.3 (3)	C22—C21—CM2	121.9 (5)
CB1—CB2—CA2	106.9 (4)	C26—C21—CM2	118.1 (4)
CB1—CB2—Br2	123.5 (3)	C21—C22—C23	119.2 (5)
CA2—CB2—Br2	129.5 (3)	C21—C22—H22	120.4
CB4—CB3—CA3	108.2 (4)	C23—C22—H22	120.4
CB4—CB3—HB3	125.9	C24—C23—C22	121.7 (5)
CA3—CB3—HB3	125.9	C24—C23—H23	119.1
CB3—CB4—CA4	109.2 (4)	C22—C23—H23	119.1
CB3—CB4—HB4	125.4	C23—C24—C25	119.5 (5)
CA4—CB4—HB4	125.4	C23—C24—H24	120.3
CA3—CM1—CA2	126.5 (4)	C25—C24—H24	120.3
CA3—CM1—C11	114.1 (4)	C24—C25—C26	120.4 (5)
CA2—CM1—C11	119.1 (4)	C24—C25—H25	119.8
CA4^{i}—CM2—CA1	126.1 (4)	C26—C25—H25	119.8
CA4^{i}—CM2—C21	114.2 (4)	C25—C26—C21	119.2 (5)
CA1—CM2—C21	119.5 (4)	C25—C26—H26	120.4
C16—C11—C12	118.9 (4)	C21—C26—H26	120.4

CA2—N1—CA1—CM2	−177.1 (4)	N1—CA2—CM1—C11	166.8 (4)
CA2—N1—CA1—CB1	−0.4 (5)	CB2—CA2—CM1—C11	−11.9 (6)
CA1—N1—CA2—CM1	−176.8 (4)	N1—CA1—CM2—CA4^{i}	−4.9 (7)
CA1—N1—CA2—CB2	2.2 (5)	CB1—CA1—CM2—CA4^{i}	179.0 (4)
CA4—N2—CA3—CM1	175.2 (5)	N1—CA1—CM2—C21	170.5 (4)
CA4—N2—CA3—CB3	−0.7 (5)	CB1—CA1—CM2—C21	−5.6 (7)
CA3—N2—CA4—CM2^{i}	−172.8 (5)	CA3—CM1—C11—C16	−74.4 (6)
CA3—N2—CA4—CB4	1.4 (5)	CA2—CM1—C11—C16	110.5 (5)
N1—CA1—CB1—CB2	−1.7 (5)	CA3—CM1—C11—C12	102.8 (5)
CM2—CA1—CB1—CB2	174.9 (4)	CA2—CM1—C11—C12	−72.3 (6)
N1—CA1—CB1—Br1	173.1 (3)	C16—C11—C12—C13	−0.2 (7)
CM2—CA1—CB1—Br1	−10.4 (7)	CM1—C11—C12—C13	−177.4 (4)
CA1—CB1—CB2—CA2	2.9 (5)	C11—C12—C13—C14	0.3 (7)
Br1—CB1—CB2—CA2	−172.4 (3)	C12—C13—C14—C15	−0.4 (8)
CA1—CB1—CB2—Br2	−172.8 (3)	C13—C14—C15—C16	0.4 (8)
Br1—CB1—CB2—Br2	11.9 (6)	C14—C15—C16—C11	−0.3 (8)
N1—CA2—CB2—CB1	−3.2 (5)	C12—C11—C16—C15	0.1 (8)
CM1—CA2—CB2—CB1	175.6 (4)	CM1—C11—C16—C15	177.3 (5)
N1—CA2—CB2—Br2	172.1 (3)	CA4^{i}—CM2—C21—C22	−74.0 (6)
CM1—CA2—CB2—Br2	−9.0 (7)	CA1—CM2—C21—C22	110.1 (5)
N2—CA3—CB3—CB4	−0.3 (5)	CA4^{i}—CM2—C21—C26	102.5 (5)
CM1—CA3—CB3—CB4	−176.5 (4)	CA1—CM2—C21—C26	−73.5 (6)
CA3—CB3—CB4—CA4	1.2 (6)	C26—C21—C22—C23	2.0 (8)
N2—CA4—CB4—CB3	−1.6 (6)	CM2—C21—C22—C23	178.4 (5)
CM2^{i}—CA4—CB4—CB3	172.8 (5)	C21—C22—C23—C24	0.7 (9)
N2—CA3—CM1—CA2	−0.3 (8)	C22—C23—C24—C25	−1.8 (9)
CB3—CA3—CM1—CA2	174.9 (4)	C23—C24—C25—C26	0.2 (9)
N2—CA3—CM1—C11	−175.0 (4)	C24—C25—C26—C21	2.5 (9)
CB3—CA3—CM1—C11	0.2 (6)	C22—C21—C26—C25	−3.5 (8)
N1—CA2—CM1—CA3	−7.6 (7)	CM2—C21—C26—C25	179.9 (5)
CB2—CA2—CM1—CA3	173.6 (4)		

Symmetry code: (i) −*x*, −*y*, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···N1	0.88	2.47	2.973 (5)	117
N2—H2···N1^{i}	0.88	2.40	2.921 (5)	118

Symmetry code: (i) −*x*, −*y*, −*z*.

(II) 7,8,17,18-Tetrabromo-5,10,15,20-tetraphenylporphyrin(2+) bis(perchlorate) dichloromethane trisolvate

Crystal data

$C_{44}H_{28}Br_4N_4^{2+}·2ClO_4^-·3CH_2Cl_2$
M_r = 1386.02
Monoclinic, *Pn*
a = 12.903 (3) Å
b = 13.761 (3) Å
c = 14.876 (3) Å
β = 96.67 (3)°
V = 2623.5 (10) Å^3

$Z = 2$
$F(000) = 1368$
$D_x = 1.755$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 250 reflections

$\theta = 1.1$–$20.5°$
$\mu = 3.53$ mm^{-1}
$T = 130$ K
Prism, blue-green
0.33 × 0.17 × 0.06 mm

Data collection

Enraf–Nonius fast area-detector diffractometer
Radiation source: ROTATING ANODE
Graphite monochromator
Detector resolution: 8.53 pixels mm^{-1}
ELLIPSOID–MASK FITTING scans
Absorption correction: part of the refinement model (ΔF)
(DIFABS; Walker & Stuart, 1983)

$T_{min} = 0.65$, $T_{max} = 1.00$
11251 measured reflections
11251 independent reflections
8745 reflections with $I > 2\sigma(I)$
$\theta_{max} = 30.0°$, $\theta_{min} = 2.5°$
$h = -16 \rightarrow 16$
$k = 0 \rightarrow 19$
$l = -19 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.060$
$wR(F^2) = 0.185$
$S = 1.06$
11251 reflections
640 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0886P)^2 + 17.5195P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.03$ e Å^{-3}
$\Delta\rho_{min} = -1.05$ e Å^{-3}
Absolute structure: Classical Flack method preferred over Parsons because s.u. lower (Flack, 1983)
Absolute structure parameter: −0.032 (14)

Special details

Experimental. Diffraction data were measured with an Enraf-Nonius FAST area detector to 55.56 deg in 2 theta. With the hardware and software supplied for the diffractometer, the data collection process provides substantial redundancy but not necessarily completion up to the limiting resolution. At a resolution of 0.83 Å (52 deg in 2 theta) essentially full coverage of data were met. Successful and suitable refinement of the structure supports this.

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.21338 (9)	1.56160 (8)	0.81718 (9)	0.0297 (3)
Br2	−0.02997 (9)	1.55748 (8)	0.89049 (9)	0.0301 (3)
Br3	0.03558 (8)	0.82412 (7)	0.99749 (8)	0.0252 (3)
Br4	0.28295 (8)	0.82050 (7)	0.92686 (8)	0.0265 (3)
N1	0.1827 (7)	1.3717 (6)	1.0200 (7)	0.0230 (19)
H1	0.2019	1.3221	1.0555	0.028*
N2	0.0484 (7)	1.2123 (6)	1.0839 (6)	0.0204 (18)
H2	0.0886	1.2076	1.0402	0.024*
N3	0.2148 (7)	1.0609 (6)	1.0661 (6)	0.0167 (16)

H3	0.2260	1.1203	1.0869	0.020*
N4	0.3381 (7)	1.2157 (6)	0.9795 (7)	0.0222 (19)
H4	0.2697	1.2093	0.9724	0.027*
CA1	0.2450 (8)	1.4179 (7)	0.9635 (8)	0.022 (2)
CA2	0.0851 (8)	1.4144 (7)	1.0124 (8)	0.020 (2)
CA3	0.0030 (8)	1.2964 (7)	1.1094 (8)	0.019 (2)
CA4	0.0213 (8)	1.1366 (7)	1.1364 (7)	0.0183 (19)
CA5	0.1262 (8)	1.0075 (7)	1.0743 (8)	0.0193 (19)
CA6	0.2834 (8)	1.0081 (7)	1.0211 (7)	0.0178 (19)
CA7	0.4088 (8)	1.1407 (7)	0.9972 (8)	0.022 (2)
CA8	0.3906 (8)	1.3014 (7)	0.9749 (8)	0.021 (2)
CB1	0.1808 (9)	1.4904 (8)	0.9173 (8)	0.025 (2)
CB2	0.0831 (8)	1.4884 (7)	0.9456 (9)	0.023 (2)
C11	−0.0765 (10)	1.4564 (8)	1.0813 (9)	0.027 (2)
CB3	−0.0511 (8)	1.2742 (6)	1.1835 (8)	0.018 (2)
HB3	−0.0902	1.3188	1.2147	0.021*
C12	−0.0536 (10)	1.5524 (8)	1.1070 (9)	0.029 (3)
H12	0.0171	1.5727	1.1175	0.035*
CB4	−0.0378 (8)	1.1765 (7)	1.2033 (8)	0.020 (2)
HB4	−0.0630	1.1425	1.2518	0.024*
C13	−0.1339 (12)	1.6199 (9)	1.1176 (11)	0.038 (3)
H13	−0.1173	1.6847	1.1358	0.045*
CB5	0.1381 (7)	0.9188 (7)	1.0280 (7)	0.0163 (18)
C14	−0.2362 (13)	1.5906 (11)	1.1012 (12)	0.044 (4)
H14	−0.2905	1.6356	1.1082	0.052*
CB6	0.2333 (9)	0.9172 (7)	0.9968 (8)	0.022 (2)
C15	−0.2605 (11)	1.4969 (10)	1.0750 (11)	0.039 (3)
H15	−0.3316	1.4778	1.0640	0.047*
CB7	0.5103 (8)	1.1810 (7)	1.0048 (8)	0.019 (2)
HB7	0.5738	1.1459	1.0165	0.023*
C16	−0.1826 (10)	1.4296 (9)	1.0642 (10)	0.031 (3)
H16	−0.2008	1.3653	1.0453	0.037*
CB8	0.5011 (8)	1.2787 (8)	0.9925 (8)	0.023 (2)
HB8	0.5569	1.3240	0.9949	0.028*
CM1	0.0064 (9)	1.3882 (7)	1.0662 (8)	0.021 (2)
CM2	0.0454 (8)	1.0384 (7)	1.1241 (7)	0.0180 (19)
CM3	0.3822 (9)	1.0421 (8)	1.0052 (8)	0.023 (2)
CM4	0.3474 (9)	1.3949 (7)	0.9573 (8)	0.022 (2)
C21	−0.0149 (9)	0.9650 (7)	1.1696 (8)	0.023 (2)
C22	−0.1224 (9)	0.9712 (8)	1.1722 (9)	0.026 (2)
H22	−0.1601	1.0230	1.1416	0.031*
C23	−0.1751 (10)	0.9040 (9)	1.2179 (10)	0.032 (3)
H23	−0.2481	0.9103	1.2202	0.038*
C24	−0.1207 (11)	0.8276 (8)	1.2602 (10)	0.031 (3)
H24	−0.1567	0.7800	1.2909	0.038*
C25	−0.0156 (12)	0.8192 (8)	1.2585 (10)	0.032 (3)
H25	0.0203	0.7661	1.2887	0.039*
C26	0.0404 (9)	0.8866 (7)	1.2135 (8)	0.022 (2)

H26	0.1136	0.8800	1.2125	0.026*
C31	0.4696 (9)	0.9730 (7)	0.9965 (8)	0.021 (2)
C32	0.5005 (9)	0.9087 (7)	1.0679 (9)	0.026 (2)
H32	0.4619	0.9049	1.1184	0.031*
C33	0.5880 (9)	0.8506 (8)	1.0642 (9)	0.026 (2)
H33	0.6103	0.8077	1.1126	0.031*
C34	0.6427 (8)	0.8558 (8)	0.9893 (10)	0.028 (3)
H34	0.7027	0.8163	0.9871	0.033*
C35	0.6114 (9)	0.9172 (8)	0.9182 (10)	0.028 (3)
H35	0.6485	0.9183	0.8666	0.034*
C36	0.5244 (9)	0.9785 (7)	0.9218 (9)	0.024 (2)
H36	0.5037	1.0226	0.8740	0.029*
C41	0.4185 (9)	1.4724 (7)	0.9340 (9)	0.025 (2)
C42	0.4811 (10)	1.4640 (8)	0.8651 (9)	0.028 (3)
H42	0.4788	1.4062	0.8299	0.034*
C43	0.5470 (10)	1.5388 (9)	0.8468 (10)	0.031 (3)
H43	0.5915	1.5309	0.8007	0.038*
C44	0.5490 (9)	1.6256 (8)	0.8951 (10)	0.030 (3)
H44	0.5921	1.6778	0.8804	0.036*
C45	0.4872 (11)	1.6347 (8)	0.9650 (11)	0.037 (3)
H45	0.4896	1.6930	0.9994	0.044*
C46	0.4211 (9)	1.5588 (7)	0.9858 (10)	0.030 (3)
H46	0.3789	1.5654	1.0337	0.036*
Cl1	0.0799 (2)	1.22478 (18)	0.8343 (2)	0.0237 (5)
O11	0.1277 (7)	1.1716 (5)	0.9135 (6)	0.0240 (16)
O12	0.1604 (8)	1.2791 (7)	0.7995 (8)	0.041 (2)
O13	0.0358 (9)	1.1571 (7)	0.7677 (7)	0.045 (3)
O14	0.0026 (8)	1.2868 (8)	0.8638 (8)	0.046 (3)
Cl2	0.2813 (2)	1.26950 (19)	1.2481 (2)	0.0262 (6)
O21	0.2935 (8)	1.2403 (7)	1.1561 (7)	0.036 (2)
O22	0.3723 (8)	1.2469 (10)	1.3065 (9)	0.055 (3)
O23	0.1930 (9)	1.2212 (9)	1.2770 (8)	0.050 (3)
O24	0.2607 (13)	1.3723 (8)	1.2457 (11)	0.071 (4)
Cl21	−0.2688 (4)	1.3297 (5)	0.6411 (4)	0.0755 (15)
Cl22	−0.2737 (5)	1.3405 (5)	0.8337 (4)	0.0818 (17)
C20	−0.201 (2)	1.357 (3)	0.7458 (17)	0.110 (11)
H20A	−0.1377	1.3155	0.7555	0.132*
H20B	−0.1771	1.4256	0.7455	0.132*
Cl31	0.6956 (2)	1.2315 (2)	1.1840 (2)	0.0347 (7)
Cl32	0.5739 (4)	1.0744 (3)	1.2483 (3)	0.0546 (11)
C30	0.5833 (10)	1.2005 (9)	1.2365 (9)	0.030 (3)
H30A	0.5874	1.2315	1.2968	0.037*
H30B	0.5201	1.2252	1.1994	0.037*
Cl41	−0.1911 (3)	1.0330 (4)	0.7629 (3)	0.0619 (12)
Cl42	−0.1778 (4)	1.1044 (4)	0.9474 (4)	0.0691 (13)
C40	−0.1286 (14)	1.0241 (13)	0.8713 (14)	0.056 (5)
H40A	−0.0534	1.0373	0.8702	0.068*
H40B	−0.1357	0.9567	0.8932	0.068*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0310 (6)	0.0282 (5)	0.0307 (7)	0.0011 (4)	0.0075 (5)	0.0114 (5)
Br2	0.0270 (6)	0.0289 (5)	0.0346 (8)	0.0086 (4)	0.0039 (5)	0.0105 (5)
Br3	0.0235 (5)	0.0230 (5)	0.0293 (7)	−0.0065 (4)	0.0046 (5)	−0.0061 (4)
Br4	0.0252 (5)	0.0233 (5)	0.0317 (7)	−0.0004 (4)	0.0056 (5)	−0.0104 (4)
N1	0.025 (4)	0.016 (4)	0.027 (6)	0.000 (3)	−0.002 (4)	0.004 (3)
N2	0.026 (4)	0.020 (4)	0.018 (5)	0.004 (3)	0.012 (4)	0.002 (3)
N3	0.015 (4)	0.017 (3)	0.020 (5)	0.000 (3)	0.005 (3)	0.000 (3)
N4	0.020 (4)	0.021 (4)	0.025 (6)	0.000 (3)	0.002 (4)	0.004 (3)
CA1	0.016 (5)	0.017 (4)	0.033 (7)	−0.009 (3)	0.006 (4)	0.002 (4)
CA2	0.018 (5)	0.019 (4)	0.025 (6)	0.001 (3)	0.003 (4)	0.000 (4)
CA3	0.018 (4)	0.019 (4)	0.020 (6)	−0.002 (3)	0.006 (4)	−0.003 (4)
CA4	0.021 (5)	0.019 (4)	0.015 (6)	−0.002 (3)	0.003 (4)	0.002 (4)
CA5	0.020 (5)	0.022 (4)	0.016 (6)	0.002 (4)	0.001 (4)	−0.001 (4)
CA6	0.018 (4)	0.020 (4)	0.016 (6)	0.004 (3)	0.003 (4)	0.004 (4)
CA7	0.020 (5)	0.015 (4)	0.031 (7)	0.000 (3)	0.006 (4)	−0.003 (4)
CA8	0.018 (5)	0.017 (4)	0.027 (7)	−0.006 (3)	0.001 (4)	−0.004 (4)
CB1	0.032 (6)	0.025 (5)	0.019 (6)	−0.003 (4)	0.005 (5)	0.004 (4)
CB2	0.013 (4)	0.020 (4)	0.036 (7)	−0.003 (3)	0.005 (4)	0.008 (4)
C11	0.037 (6)	0.019 (5)	0.025 (7)	−0.001 (4)	0.006 (5)	−0.004 (4)
CB3	0.018 (4)	0.014 (4)	0.022 (6)	0.006 (3)	0.002 (4)	−0.002 (3)
C12	0.029 (6)	0.026 (5)	0.032 (8)	−0.007 (4)	0.005 (5)	−0.009 (5)
CB4	0.022 (5)	0.019 (5)	0.021 (6)	0.003 (3)	0.007 (4)	−0.003 (4)
C13	0.045 (7)	0.024 (5)	0.044 (9)	0.012 (5)	0.008 (6)	−0.013 (5)
CB5	0.015 (4)	0.017 (4)	0.017 (6)	−0.005 (3)	0.001 (4)	−0.003 (3)
C14	0.046 (8)	0.038 (7)	0.048 (10)	0.015 (6)	0.010 (7)	−0.005 (6)
CB6	0.027 (5)	0.014 (4)	0.026 (6)	0.004 (4)	0.006 (4)	0.006 (4)
C15	0.034 (7)	0.041 (7)	0.043 (9)	0.008 (5)	0.004 (6)	0.002 (6)
CB7	0.017 (5)	0.020 (4)	0.019 (6)	−0.001 (3)	−0.002 (4)	0.002 (4)
C16	0.027 (6)	0.035 (6)	0.029 (8)	0.002 (5)	0.001 (5)	−0.003 (5)
CB8	0.016 (5)	0.027 (5)	0.026 (7)	−0.003 (4)	0.003 (4)	0.005 (4)
CM1	0.028 (5)	0.019 (4)	0.016 (6)	−0.002 (4)	0.004 (4)	−0.003 (4)
CM2	0.022 (5)	0.022 (4)	0.010 (5)	−0.001 (4)	0.006 (4)	−0.001 (3)
CM3	0.023 (5)	0.025 (5)	0.022 (6)	−0.001 (4)	0.005 (4)	0.005 (4)
CM4	0.024 (5)	0.019 (4)	0.026 (7)	−0.001 (4)	0.010 (4)	−0.004 (4)
C21	0.022 (5)	0.023 (5)	0.025 (7)	−0.006 (4)	0.011 (4)	−0.005 (4)
C22	0.026 (6)	0.029 (5)	0.024 (7)	−0.007 (4)	0.005 (5)	−0.004 (4)
C23	0.021 (5)	0.042 (6)	0.033 (8)	−0.016 (5)	0.006 (5)	−0.007 (5)
C24	0.042 (7)	0.029 (6)	0.024 (7)	−0.013 (5)	0.006 (5)	0.002 (5)
C25	0.049 (8)	0.024 (5)	0.027 (8)	−0.014 (5)	0.015 (6)	0.001 (4)
C26	0.029 (5)	0.018 (4)	0.016 (6)	−0.003 (4)	−0.006 (4)	−0.002 (4)
C31	0.023 (5)	0.017 (4)	0.023 (6)	−0.005 (4)	−0.001 (4)	−0.005 (4)
C32	0.034 (6)	0.013 (4)	0.030 (7)	0.000 (4)	0.003 (5)	0.006 (4)
C33	0.026 (5)	0.019 (4)	0.033 (7)	0.002 (4)	0.004 (5)	0.003 (4)
C34	0.017 (5)	0.020 (5)	0.046 (8)	0.001 (4)	0.003 (5)	−0.006 (5)
C35	0.022 (5)	0.024 (5)	0.041 (8)	0.006 (4)	0.010 (5)	−0.009 (5)

C36	0.025 (5)	0.020 (4)	0.027 (7)	0.006 (4)	0.007 (4)	0.004 (4)
C41	0.022 (5)	0.020 (5)	0.032 (7)	0.004 (4)	0.004 (5)	0.006 (4)
C42	0.034 (6)	0.023 (5)	0.030 (7)	0.001 (4)	0.009 (5)	0.004 (4)
C43	0.025 (6)	0.038 (6)	0.032 (8)	−0.001 (5)	0.004 (5)	0.005 (5)
C44	0.029 (6)	0.023 (5)	0.036 (8)	−0.007 (4)	−0.011 (5)	0.013 (5)
C45	0.042 (7)	0.019 (5)	0.049 (9)	−0.012 (5)	0.005 (6)	−0.001 (5)
C46	0.025 (5)	0.018 (5)	0.047 (8)	−0.003 (4)	0.007 (5)	−0.002 (5)
Cl1	0.0233 (12)	0.0263 (11)	0.0214 (16)	0.0024 (9)	0.0024 (10)	−0.0023 (9)
O11	0.034 (4)	0.022 (4)	0.015 (4)	0.001 (3)	0.000 (3)	−0.002 (3)
O12	0.038 (5)	0.040 (5)	0.046 (7)	−0.005 (4)	0.014 (5)	0.014 (4)
O13	0.064 (7)	0.038 (5)	0.030 (6)	−0.007 (5)	−0.008 (5)	−0.012 (4)
O14	0.031 (5)	0.069 (7)	0.039 (7)	0.027 (5)	0.003 (4)	−0.006 (5)
Cl2	0.0264 (12)	0.0276 (12)	0.0252 (16)	−0.0027 (10)	0.0049 (11)	−0.0046 (10)
O21	0.049 (6)	0.033 (4)	0.027 (6)	−0.001 (4)	0.009 (4)	−0.001 (4)
O22	0.027 (5)	0.092 (9)	0.045 (8)	0.010 (5)	−0.003 (5)	−0.003 (6)
O23	0.038 (6)	0.067 (7)	0.046 (7)	−0.016 (5)	0.011 (5)	0.006 (5)
O24	0.111 (12)	0.032 (5)	0.075 (10)	0.011 (6)	0.039 (9)	−0.009 (6)
Cl21	0.055 (3)	0.124 (5)	0.046 (3)	−0.012 (3)	−0.002 (2)	0.004 (3)
Cl22	0.067 (3)	0.131 (5)	0.047 (3)	0.025 (3)	0.006 (2)	−0.015 (3)
C20	0.078 (17)	0.21 (3)	0.034 (15)	−0.017 (19)	−0.016 (11)	0.014 (17)
Cl31	0.0267 (14)	0.0446 (16)	0.0337 (19)	−0.0082 (12)	0.0071 (12)	−0.0090 (13)
Cl32	0.059 (2)	0.0410 (18)	0.068 (3)	−0.0209 (16)	0.024 (2)	−0.0156 (18)
C30	0.030 (6)	0.034 (6)	0.028 (7)	−0.005 (5)	0.009 (5)	−0.006 (5)
Cl41	0.036 (2)	0.105 (4)	0.044 (3)	0.005 (2)	−0.0038 (17)	−0.008 (2)
Cl42	0.070 (3)	0.087 (3)	0.049 (3)	−0.023 (3)	0.002 (2)	−0.008 (2)
C40	0.047 (9)	0.054 (9)	0.065 (13)	0.004 (7)	−0.009 (8)	0.012 (8)

Geometric parameters (Å, º)

Br1—CB1	1.872 (11)	CM4—C41	1.475 (14)
Br2—CB2	1.851 (11)	C21—C22	1.395 (16)
Br3—CB5	1.874 (9)	C21—C26	1.411 (16)
Br4—CB6	1.849 (11)	C22—C23	1.373 (16)
N1—CA2	1.383 (13)	C22—H22	0.9500
N1—CA1	1.383 (13)	C23—C24	1.38 (2)
N1—H1	0.8807	C23—H23	0.9500
N2—CA3	1.369 (12)	C24—C25	1.36 (2)
N2—CA4	1.372 (13)	C24—H24	0.9500
N2—H2	0.8799	C25—C26	1.393 (15)
N3—CA5	1.377 (13)	C25—H25	0.9500
N3—CA6	1.377 (12)	C26—H26	0.9500
N3—H3	0.8800	C31—C36	1.386 (16)
N4—CA8	1.365 (12)	C31—C32	1.404 (16)
N4—CA7	1.382 (13)	C32—C33	1.389 (15)
N4—H4	0.8810	C32—H32	0.9500
CA1—CM4	1.371 (15)	C33—C34	1.387 (18)
CA1—CB1	1.422 (16)	C33—H33	0.9500
CA2—CM1	1.411 (15)	C34—C35	1.378 (19)

CA2—CB2	1.421 (15)	C34—H34	0.9500
CA3—CB3	1.405 (15)	C35—C36	1.410 (14)
CA3—CM1	1.420 (14)	C35—H35	0.9500
CA4—CM2	1.403 (14)	C36—H36	0.9500
CA4—CB4	1.432 (14)	C41—C42	1.382 (17)
CA5—CM2	1.413 (14)	C41—C46	1.415 (16)
CA5—CB5	1.419 (13)	C42—C43	1.382 (17)
CA6—CM3	1.403 (14)	C42—H42	0.9500
CA6—CB6	1.435 (15)	C43—C44	1.392 (19)
CA7—CM3	1.409 (14)	C43—H43	0.9500
CA7—CB7	1.414 (14)	C44—C45	1.39 (2)
CA8—CM4	1.414 (14)	C44—H44	0.9500
CA8—CB8	1.453 (15)	C45—C46	1.404 (15)
CB1—CB2	1.374 (15)	C45—H45	0.9500
C11—C12	1.397 (15)	C46—H46	0.9500
C11—C16	1.413 (18)	Cl1—O14	1.420 (9)
C11—CM1	1.460 (15)	Cl1—O12	1.425 (9)
CB3—CB4	1.382 (13)	Cl1—O13	1.429 (10)
CB3—HB3	0.9500	Cl1—O11	1.461 (9)
C12—C13	1.413 (17)	Cl2—O22	1.411 (12)
C12—H12	0.9500	Cl2—O23	1.428 (10)
CB4—HB4	0.9500	Cl2—O24	1.439 (11)
C13—C14	1.37 (2)	Cl2—O21	1.453 (10)
C13—H13	0.9500	Cl21—C20	1.74 (3)
CB5—CB6	1.363 (14)	Cl22—C20	1.71 (3)
C14—C15	1.37 (2)	C20—H20A	0.9900
C14—H14	0.9500	C20—H20B	0.9900
C15—C16	1.390 (18)	Cl31—C30	1.776 (12)
C15—H15	0.9500	Cl32—C30	1.749 (13)
CB7—CB8	1.361 (14)	C30—H30A	0.9900
CB7—HB7	0.9500	C30—H30B	0.9900
C16—H16	0.9500	Cl41—C40	1.72 (2)
CB8—HB8	0.9500	Cl42—C40	1.75 (2)
CM2—C21	1.485 (14)	C40—H40A	0.9900
CM3—C31	1.493 (15)	C40—H40B	0.9900

CA2—N1—CA1	110.1 (9)	CA1—CM4—CA8	124.0 (9)
CA2—N1—H1	124.6	CA1—CM4—C41	118.6 (9)
CA1—N1—H1	125.2	CA8—CM4—C41	117.4 (9)
CA3—N2—CA4	109.8 (8)	C22—C21—C26	119.0 (10)
CA3—N2—H2	125.0	C22—C21—CM2	123.1 (11)
CA4—N2—H2	125.1	C26—C21—CM2	117.9 (10)
CA5—N3—CA6	110.4 (8)	C23—C22—C21	121.6 (12)
CA5—N3—H3	124.7	C23—C22—H22	119.2
CA6—N3—H3	124.9	C21—C22—H22	119.2
CA8—N4—CA7	109.5 (9)	C22—C23—C24	119.0 (12)
CA8—N4—H4	125.2	C22—C23—H23	120.5
CA7—N4—H4	125.3	C24—C23—H23	120.5

CM4—CA1—N1	124.5 (10)	C25—C24—C23	120.8 (11)
CM4—CA1—CB1	129.9 (10)	C25—C24—H24	119.6
N1—CA1—CB1	105.5 (9)	C23—C24—H24	119.6
N1—CA2—CM1	123.6 (10)	C24—C25—C26	121.7 (13)
N1—CA2—CB2	107.7 (9)	C24—C25—H25	119.2
CM1—CA2—CB2	128.7 (10)	C26—C25—H25	119.2
N2—CA3—CB3	107.5 (8)	C25—C26—C21	117.9 (11)
N2—CA3—CM1	126.1 (9)	C25—C26—H26	121.0
CB3—CA3—CM1	126.3 (9)	C21—C26—H26	121.0
N2—CA4—CM2	125.7 (9)	C36—C31—C32	121.0 (10)
N2—CA4—CB4	107.1 (8)	C36—C31—CM3	119.7 (10)
CM2—CA4—CB4	127.2 (9)	C32—C31—CM3	119.2 (10)
N3—CA5—CM2	123.9 (9)	C33—C32—C31	119.5 (11)
N3—CA5—CB5	106.2 (8)	C33—C32—H32	120.2
CM2—CA5—CB5	129.9 (10)	C31—C32—H32	120.2
N3—CA6—CM3	123.6 (9)	C34—C33—C32	119.6 (11)
N3—CA6—CB6	106.6 (8)	C34—C33—H33	120.2
CM3—CA6—CB6	129.7 (9)	C32—C33—H33	120.2
N4—CA7—CM3	125.0 (10)	C35—C34—C33	121.2 (10)
N4—CA7—CB7	107.9 (8)	C35—C34—H34	119.4
CM3—CA7—CB7	127.1 (10)	C33—C34—H34	119.4
N4—CA8—CM4	127.4 (10)	C34—C35—C36	120.0 (11)
N4—CA8—CB8	106.7 (9)	C34—C35—H35	120.0
CM4—CA8—CB8	125.8 (9)	C36—C35—H35	120.0
CB2—CB1—CA1	110.1 (9)	C31—C36—C35	118.7 (11)
CB2—CB1—Br1	123.5 (9)	C31—C36—H36	120.6
CA1—CB1—Br1	125.4 (8)	C35—C36—H36	120.6
CB1—CB2—CA2	106.6 (9)	C42—C41—C46	119.7 (10)
CB1—CB2—Br2	123.9 (8)	C42—C41—CM4	123.2 (10)
CA2—CB2—Br2	128.8 (7)	C46—C41—CM4	117.1 (10)
C12—C11—C16	117.7 (11)	C41—C42—C43	120.7 (12)
C12—C11—CM1	121.0 (11)	C41—C42—H42	119.7
C16—C11—CM1	121.1 (10)	C43—C42—H42	119.7
CB4—CB3—CA3	108.5 (8)	C42—C43—C44	120.8 (12)
CB4—CB3—HB3	125.7	C42—C43—H43	119.6
CA3—CB3—HB3	125.7	C44—C43—H43	119.6
C11—C12—C13	121.2 (12)	C45—C44—C43	119.1 (11)
C11—C12—H12	119.4	C45—C44—H44	120.5
C13—C12—H12	119.4	C43—C44—H44	120.5
CB3—CB4—CA4	106.8 (9)	C44—C45—C46	120.9 (12)
CB3—CB4—HB4	126.6	C44—C45—H45	119.5
CA4—CB4—HB4	126.6	C46—C45—H45	119.5
C14—C13—C12	119.3 (12)	C45—C46—C41	118.8 (12)
C14—C13—H13	120.4	C45—C46—H46	120.6
C12—C13—H13	120.4	C41—C46—H46	120.6
CB6—CB5—CA5	109.4 (9)	O14—Cl1—O12	111.4 (7)
CB6—CB5—Br3	123.0 (8)	O14—Cl1—O13	111.6 (7)
CA5—CB5—Br3	127.1 (7)	O12—Cl1—O13	109.7 (7)

C15—C14—C13	120.6 (13)	O14—Cl1—O11	107.3 (6)
C15—C14—H14	119.7	O12—Cl1—O11	107.4 (6)
C13—C14—H14	119.7	O13—Cl1—O11	109.3 (5)
CB5—CB6—CA6	107.3 (9)	O22—Cl2—O23	110.4 (8)
CB5—CB6—Br4	126.0 (8)	O22—Cl2—O24	111.7 (9)
CA6—CB6—Br4	126.4 (8)	O23—Cl2—O24	108.3 (8)
C14—C15—C16	120.9 (14)	O22—Cl2—O21	110.2 (7)
C14—C15—H15	119.5	O23—Cl2—O21	109.3 (7)
C16—C15—H15	119.5	O24—Cl2—O21	106.7 (7)
CB8—CB7—CA7	108.1 (9)	Cl22—C20—Cl21	112.8 (16)
CB8—CB7—HB7	126.0	Cl22—C20—H20A	109.0
CA7—CB7—HB7	126.0	Cl21—C20—H20A	109.0
C15—C16—C11	120.3 (12)	Cl22—C20—H20B	109.0
C15—C16—H16	119.8	Cl21—C20—H20B	109.0
C11—C16—H16	119.8	H20A—C20—H20B	107.8
CB7—CB8—CA8	107.8 (9)	Cl32—C30—Cl31	110.6 (7)
CB7—CB8—HB8	126.1	Cl32—C30—H30A	109.5
CA8—CB8—HB8	126.1	Cl31—C30—H30A	109.5
CA2—CM1—CA3	123.1 (9)	Cl32—C30—H30B	109.5
CA2—CM1—C11	120.7 (9)	Cl31—C30—H30B	109.5
CA3—CM1—C11	116.2 (9)	H30A—C30—H30B	108.1
CA4—CM2—CA5	123.1 (9)	Cl41—C40—Cl42	113.2 (10)
CA4—CM2—C21	117.4 (9)	Cl41—C40—H40A	108.9
CA5—CM2—C21	119.5 (9)	Cl42—C40—H40A	108.9
CA6—CM3—CA7	124.8 (10)	Cl41—C40—H40B	108.9
CA6—CM3—C31	120.8 (9)	Cl42—C40—H40B	108.9
CA7—CM3—C31	114.4 (9)	H40A—C40—H40B	107.7

CA2—N1—CA1—CM4	177.8 (11)	CB3—CA3—CM1—C11	−19.5 (17)
CA2—N1—CA1—CB1	−1.8 (13)	C12—C11—CM1—CA2	−48.1 (18)
CA1—N1—CA2—CM1	−175.3 (11)	C16—C11—CM1—CA2	127.4 (14)
CA1—N1—CA2—CB2	2.5 (13)	C12—C11—CM1—CA3	131.2 (13)
CA4—N2—CA3—CB3	2.7 (13)	C16—C11—CM1—CA3	−53.3 (17)
CA4—N2—CA3—CM1	−174.8 (11)	N2—CA4—CM2—CA5	19.9 (18)
CA3—N2—CA4—CM2	173.8 (11)	CB4—CA4—CM2—CA5	−162.0 (12)
CA3—N2—CA4—CB4	−4.6 (13)	N2—CA4—CM2—C21	−162.9 (11)
CA6—N3—CA5—CM2	174.2 (10)	CB4—CA4—CM2—C21	15.1 (17)
CA6—N3—CA5—CB5	−3.0 (12)	N3—CA5—CM2—CA4	29.0 (17)
CA5—N3—CA6—CM3	−177.8 (10)	CB5—CA5—CM2—CA4	−154.4 (12)
CA5—N3—CA6—CB6	2.1 (12)	N3—CA5—CM2—C21	−148.1 (11)
CA8—N4—CA7—CM3	−179.1 (11)	CB5—CA5—CM2—C21	28.5 (18)
CA8—N4—CA7—CB7	0.5 (14)	N3—CA6—CM3—CA7	−27.5 (18)
CA7—N4—CA8—CM4	179.4 (12)	CB6—CA6—CM3—CA7	152.6 (13)
CA7—N4—CA8—CB8	−1.1 (14)	N3—CA6—CM3—C31	151.6 (11)
CM4—CA1—CB1—CB2	−179.2 (12)	CB6—CA6—CM3—C31	−28.2 (19)
N1—CA1—CB1—CB2	0.4 (13)	N4—CA7—CM3—CA6	−18 (2)
CM4—CA1—CB1—Br1	12.1 (19)	CB7—CA7—CM3—CA6	162.1 (12)
N1—CA1—CB1—Br1	−168.4 (8)	N4—CA7—CM3—C31	162.4 (11)

CA1—CB1—CB2—CA2	1.1 (14)	CB7—CA7—CM3—C31	−17.1 (18)
Br1—CB1—CB2—CA2	170.1 (9)	N1—CA1—CM4—CA8	28.0 (19)
CA1—CB1—CB2—Br2	−170.3 (9)	CB1—CA1—CM4—CA8	−152.5 (13)
Br1—CB1—CB2—Br2	−1.3 (15)	N1—CA1—CM4—C41	−149.8 (11)
N1—CA2—CB2—CB1	−2.2 (13)	CB1—CA1—CM4—C41	29.6 (19)
CM1—CA2—CB2—CB1	175.5 (12)	N4—CA8—CM4—CA1	17 (2)
N1—CA2—CB2—Br2	168.6 (9)	CB8—CA8—CM4—CA1	−162.9 (13)
CM1—CA2—CB2—Br2	−13.7 (19)	N4—CA8—CM4—C41	−165.5 (12)
N2—CA3—CB3—CB4	0.4 (13)	CB8—CA8—CM4—C41	15.0 (19)
CM1—CA3—CB3—CB4	177.9 (11)	CA4—CM2—C21—C22	42.4 (16)
C16—C11—C12—C13	1 (2)	CA5—CM2—C21—C22	−140.3 (12)
CM1—C11—C12—C13	177.1 (13)	CA4—CM2—C21—C26	−136.4 (11)
CA3—CB3—CB4—CA4	−3.2 (13)	CA5—CM2—C21—C26	40.9 (16)
N2—CA4—CB4—CB3	4.8 (12)	C26—C21—C22—C23	1.4 (18)
CM2—CA4—CB4—CB3	−173.6 (11)	CM2—C21—C22—C23	−177.4 (11)
C11—C12—C13—C14	−1 (2)	C21—C22—C23—C24	−1.7 (19)
N3—CA5—CB5—CB6	2.8 (12)	C22—C23—C24—C25	1 (2)
CM2—CA5—CB5—CB6	−174.2 (11)	C23—C24—C25—C26	−1 (2)
N3—CA5—CB5—Br3	−168.8 (8)	C24—C25—C26—C21	0.3 (19)
CM2—CA5—CB5—Br3	14.2 (18)	C22—C21—C26—C25	−0.7 (17)
C12—C13—C14—C15	0 (3)	CM2—C21—C26—C25	178.2 (11)
CA5—CB5—CB6—CA6	−1.6 (13)	CA6—CM3—C31—C36	127.8 (12)
Br3—CB5—CB6—CA6	170.4 (8)	CA7—CM3—C31—C36	−53.0 (15)
CA5—CB5—CB6—Br4	−176.5 (8)	CA6—CM3—C31—C32	−57.4 (16)
Br3—CB5—CB6—Br4	−4.4 (14)	CA7—CM3—C31—C32	121.8 (12)
N3—CA6—CB6—CB5	−0.3 (12)	C36—C31—C32—C33	0.8 (17)
CM3—CA6—CB6—CB5	179.6 (11)	CM3—C31—C32—C33	−173.9 (10)
N3—CA6—CB6—Br4	174.6 (8)	C31—C32—C33—C34	−1.1 (17)
CM3—CA6—CB6—Br4	−5.5 (18)	C32—C33—C34—C35	−0.3 (17)
C13—C14—C15—C16	0 (3)	C33—C34—C35—C36	2.0 (18)
N4—CA7—CB7—CB8	0.3 (14)	C32—C31—C36—C35	0.8 (17)
CM3—CA7—CB7—CB8	179.9 (12)	CM3—C31—C36—C35	175.5 (10)
C14—C15—C16—C11	1 (2)	C34—C35—C36—C31	−2.2 (17)
C12—C11—C16—C15	−1 (2)	CA1—CM4—C41—C42	−128.5 (13)
CM1—C11—C16—C15	−177.1 (13)	CA8—CM4—C41—C42	53.5 (18)
CA7—CB7—CB8—CA8	−1.0 (14)	CA1—CM4—C41—C46	51.5 (17)
N4—CA8—CB8—CB7	1.3 (14)	CA8—CM4—C41—C46	−126.5 (12)
CM4—CA8—CB8—CB7	−179.2 (11)	C46—C41—C42—C43	1 (2)
N1—CA2—CM1—CA3	−23.0 (18)	CM4—C41—C42—C43	−179.4 (12)
CB2—CA2—CM1—CA3	159.7 (12)	C41—C42—C43—C44	−2 (2)
N1—CA2—CM1—C11	156.2 (11)	C42—C43—C44—C45	3 (2)
CB2—CA2—CM1—C11	−21.1 (19)	C43—C44—C45—C46	−2 (2)
N2—CA3—CM1—CA2	−23.3 (19)	C44—C45—C46—C41	0 (2)
CB3—CA3—CM1—CA2	159.7 (11)	C42—C41—C46—C45	0.5 (19)
N2—CA3—CM1—C11	157.5 (11)	CM4—C41—C46—C45	−179.5 (12)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N2	0.88	2.57	3.018 (12)	113
N1—H1···O21	0.88	2.12	2.956 (14)	158
N2—H2···N1	0.88	2.60	3.018 (12)	110
N2—H2···N3	0.88	2.59	3.026 (12)	111
N2—H2···O11	0.88	2.07	2.896 (12)	157
N3—H3···O21	0.88	2.08	2.932 (13)	162
N4—H4···N3	0.88	2.62	3.034 (12)	110
N4—H4···O11	0.88	2.01	2.844 (13)	159