1,8-bis(2-hydroxy-3,5-di-*tert*-butylbenzyl)-4,11-dibenzyl-1,4,8,11-tetraazacyclotetradecane

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SUPPLEMENTARY INFORMATION

Table S1. X-ray diffraction experimental data

Chemical formula	$C_{54}H_{80}N_4O_2$
M_r	817.22
Crystal system, space group	Triclinic, *P*-1
Temperature (K)	123
a, *b*, *c* (Å)	8.4026 (6), 11.8152 (8), 13.3515 (10)
α, β, γ (°)	109.180 (7), 98.602 (6), 97.535 (6)
V (Å^3)	1214.57 (15)
Z	1
Radiation type	Mo*K*α
μ (mm^{-1})	0.07
Crystal size (mm)	0.3 × 0.2 × 0.05
Data collection	
Diffractometer	Xcalibur
Absorption correction	Analytical *CrysAlis PRO*, Agilent Technologies,Version 1.171.37.35 (release 13-08-2014 CrysAlis171 .NET) (compiled Aug 13 2014,18:06:01) Analytical numeric absorption correction using a multifaceted crystal model based on expressions derived by R.C. Clark & J.S. Reid. (Clark, R. C. & Reid, J. S. (1995). Acta Cryst. A51, 887-897) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min}, T_{max}	0.984, 0.997
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9706, 4248, 3168
R_{int}	0.038
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.595

Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.062, 0.136, 1.04
No. of reflections	4248
No. of parameters	281
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$(e Å^{-3})	0.25, −0.17

Computer programs: *CrysAlis PRO*, *SHELXS97* (Sheldrick, 1990), *SHELXL97* (Sheldrick, 1997), *X-SEED*.

Table S2. X-ray diffraction crystal data

$C_{54}H_{80}N_4O_2$	Z = 1
M_r = 817.22	F(000) = 448
Triclinic, $P\bar{1}$	D_x = 1.117 Mg m^{-3}
a = 8.4026 (6) Å	Mo $K\alpha$ radiation, λ = 0.71073 Å
b = 11.8152 (8) Å	Cell parameters from 9830 reflections
c = 13.3515 (10) Å	θ = 3.0–26.4°
α = 109.180 (7)°	μ = 0.07 mm^{-1}
β = 98.602 (6)°	T = 123 K
γ = 97.535 (6)°	Plate, colourless
V = 1214.57 (15) Å^3	0.3 × 0.2 × 0.05 mm

Table S3. Data Collection

Xcalibur diffractometer	4248 independent reflections
Radiation source: fine-focus sealed tube	3168 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.038$
scans in phi and ω	$\theta_{max} = 25.0°$, $\theta_{min} = 3.2°$
Absorption correction: analytical *CrysAlis PRO*, Agilent Technologies, Version 1.171.37.35 (release 13-08-2014 CrysAlis171 .NET) (compiled Aug 13 2014,18:06:01) Analytical numeric absorption correction using a multifaceted crystal model based on expressions derived by R.C. Clark & J.S. Reid. (Clark, R. C. & Reid, J. S. (1995). Acta Cryst. A51, 887-897) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	$h = -9 \rightarrow 9$
$T_{min} = 0.984$, $T_{max} = 0.997$	$k = -13 \rightarrow 14$
9706 measured reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.062$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.136$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.04$	$W = 1/[\sigma^2(F_o^2) + (0.0519P)^2 + 0.4735P]$ where $P = (F_o^2 + 2F_c^2)/3$
4248 reflections	$(\Delta/\sigma)_{max} < 0.001$
281 parameters	$\Delta\rho_{max} = 0.25$ e Å^{-3}
1 restraint	$\Delta\rho_{min} = -0.17$ e Å^{-3}

Special details regarding X-ray diffraction

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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. The structure was solved by direct methods. The asymmetric unit contains half the molecule (inversion symmetry). All non H-atoms are refined anisotropically. The H-atoms are placed in calculated positions except for H1 which was found. The thermal parameter was fixed to 1.2 times that of the parent atom and the O1—H1 bond length is restrained (*DFIX*) to 0.95 A.

Table S4. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	X	y	z	U_{iso}*/U_{eq}
O1	0.79450 (18)	0.60786 (14)	0.36494 (13)	0.0278 (4)
N1	1.2471 (2)	0.66286 (16)	0.66519 (15)	0.0251 (4)
N2	1.0504 (2)	0.47245 (15)	0.31728 (14)	0.0222 (4)
C1	1.1378 (3)	0.72753 (19)	0.72805 (19)	0.0268 (5)
H1A	1.1375	0.8064	0.7171	0.032*
H1B	1.1815	0.7457	0.8059	0.032*
C2	1.2025 (3)	0.6494 (2)	0.55058 (18)	0.0274 (5)
H2A	1.2305	0.7305	0.5441	0.033*
H2B	1.0823	0.6212	0.5256	0.033*
C3	1.2871 (3)	0.5608 (2)	0.47700 (18)	0.0270 (5)
H3A	1.2707	0.4825	0.4896	0.032*
H3B	1.4064	0.5942	0.4953	0.032*
C4	1.2221 (3)	0.5375 (2)	0.35824 (18)	0.0258 (5)
H4A	1.2318	0.6169	0.3474	0.031*
H4B	1.2920	0.4893	0.3147	0.031*
C5	1.0387 (3)	0.34301 (19)	0.30143 (19)	0.0265 (5)
H5A	1.0954	0.3354	0.3688	0.032*
H5B	1.0963	0.3055	0.2431	0.032*
C6	1.4180 (3)	0.7281 (2)	0.71289 (19)	0.0334 (6)
H6A	1.4247	0.8153	0.7219	0.040*
H6B	1.4889	0.6941	0.6621	0.040*
C7	1.4822 (3)	0.7189 (2)	0.82112 (19)	0.0294 (5)
C8	1.5318 (3)	0.8206 (2)	0.9152 (2)	0.0380 (6)
H8	1.5212	0.8990	0.9132	0.046*
C9	1.5970 (3)	0.8091 (3)	1.0126 (2)	0.0440 (7)

H9	1.6311	0.8797	1.0765	0.053*
C10	1.6126 (3)	0.6967 (3)	1.0174 (2)	0.0452 (7)
H10	1.6578	0.6893	1.0840	0.054*
C11	1.5619 (3)	0.5947 (3)	0.9241 (2)	0.0440 (7)
H11	1.5725	0.5165	0.9265	0.053*
C12	1.4960 (3)	0.6055 (2)	0.8276 (2)	0.0336 (6)
H12	1.4595	0.5342	0.7644	0.040*
C13	0.9831 (3)	0.49069 (19)	0.21700 (17)	0.0247 (5)
H13A	0.8753	0.4353	0.1832	0.030*
H13B	1.0573	0.4691	0.1656	0.030*
C14	0.9623 (3)	0.62031 (19)	0.23697 (17)	0.0219 (5)
C15	0.8654 (3)	0.67318 (19)	0.30952 (17)	0.0226 (5)
C16	0.8363 (2)	0.79139 (18)	0.32567 (17)	0.0214 (5)
C17	0.9149 (2)	0.85521 (19)	0.26949 (17)	0.0215 (5)
H17	0.8970	0.9355	0.2793	0.026*
C18	1.0175 (2)	0.80842 (19)	0.20026 (17)	0.0217 (5)
C19	1.0376 (3)	0.68937 (19)	0.18442 (17)	0.0240 (5)
H19	1.1049	0.6541	0.1362	0.029*
C20	0.7206 (3)	0.84670 (19)	0.39911 (18)	0.0251 (5)
C21	0.7870 (3)	0.8591 (2)	0.51612 (19)	0.0390 (6)
H21A	0.8912	0.9178	0.5443	0.058*
H21B	0.8045	0.7795	0.5183	0.058*
H21C	0.7077	0.8880	0.5608	0.058*
C22	0.5496 (3)	0.7637 (2)	0.3586 (2)	0.0334 (6)
H22A	0.5568	0.6841	0.3649	0.050*
H22B	0.5091	0.7526	0.2826	0.050*
H22C	0.4740	0.8015	0.4024	0.050*
C23	0.7007 (3)	0.9736 (2)	0.3985 (2)	0.0353 (6)

H23A	0.6233	1.0043	0.4441	0.053*
H23B	0.6588	0.9680	0.3241	0.053*
H23C	0.8073	1.0294	0.4268	0.053*
C24	1.1096 (3)	0.8822 (2)	0.14376 (18)	0.0267 (5)
C25	1.0620 (3)	1.0068 (2)	0.1626 (2)	0.0333 (6)
H25A	1.1243	1.0505	0.1255	0.050*
H25B	1.0868	1.0543	0.2405	0.050*
H25C	0.9444	0.9957	0.1340	0.050*
C26	1.0752 (3)	0.8126 (2)	0.02160 (19)	0.0399 (6)
H26A	0.9569	0.7956	−0.0075	0.060*
H26B	1.1146	0.7355	0.0073	0.060*
H26C	1.1321	0.8621	−0.0133	0.060*
C27	1.2937 (3)	0.9027 (2)	0.1894 (2)	0.0388 (6)
H27A	1.3544	0.9528	0.1566	0.058*
H27B	1.3286	0.8237	0.1726	0.058*
H27C	1.3160	0.9447	0.2681	0.058*
H1	0.839 (4)	0.5362 (18)	0.355 (3)	0.085 (11)*

Table S5. X-ray diffraction atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0328 (9)	0.0265 (9)	0.0318 (10)	0.0087 (7)	0.0142 (7)	0.0159 (8)
N1	0.0227 (10)	0.0278 (10)	0.0249 (11)	0.0024 (8)	0.0045 (8)	0.0105 (9)
N2	0.0237 (10)	0.0212 (10)	0.0248 (10)	0.0047 (7)	0.0048 (8)	0.0122 (8)
C1	0.0338 (13)	0.0196 (12)	0.0292 (13)	0.0067 (10)	0.0091 (11)	0.0097 (10)
C2	0.0276 (13)	0.0269 (13)	0.0302 (14)	0.0034 (10)	0.0055 (10)	0.0142 (11)
C3	0.0221 (12)	0.0314 (13)	0.0315 (14)	0.0056 (10)	0.0063 (10)	0.0160 (11)
C4	0.0221 (12)	0.0309 (13)	0.0280 (13)	0.0042 (9)	0.0088 (10)	0.0138 (11)
C5	0.0319 (13)	0.0247 (12)	0.0286 (13)	0.0106 (10)	0.0115 (10)	0.0127 (11)
C6	0.0302 (14)	0.0345 (14)	0.0318 (14)	−0.0049 (10)	0.0058 (11)	0.0114 (12)
C7	0.0220 (12)	0.0363 (14)	0.0265 (13)	−0.0012 (10)	0.0052 (10)	0.0092 (12)
C8	0.0308 (14)	0.0353 (15)	0.0398 (16)	−0.0022 (11)	0.0048 (12)	0.0070 (13)
C9	0.0329 (15)	0.0557 (19)	0.0263 (15)	−0.0061 (12)	0.0006 (11)	0.0003 (13)
C10	0.0329 (15)	0.068 (2)	0.0326 (16)	0.0014 (13)	0.0003 (12)	0.0216 (15)
C11	0.0386 (16)	0.0511 (17)	0.0446 (18)	0.0060 (13)	0.0035 (13)	0.0233 (15)
C12	0.0287 (13)	0.0379 (15)	0.0298 (14)	0.0026 (11)	0.0062 (11)	0.0078 (12)
C13	0.0287 (13)	0.0239 (12)	0.0220 (13)	0.0055 (9)	0.0055 (10)	0.0085 (10)
C14	0.0230 (12)	0.0233 (12)	0.0184 (12)	0.0032 (9)	0.0002 (9)	0.0083 (10)
C15	0.0206 (11)	0.0251 (12)	0.0220 (12)	0.0013 (9)	0.0013 (9)	0.0109 (10)
C16	0.0188 (11)	0.0216 (12)	0.0210 (12)	0.0015 (9)	0.0010 (9)	0.0060 (10)
C17	0.0226 (12)	0.0186 (11)	0.0223 (12)	0.0046 (9)	−0.0001 (9)	0.0078 (10)
C18	0.0217 (12)	0.0255 (12)	0.0181 (12)	0.0036 (9)	0.0007 (9)	0.0099 (10)
C19	0.0236 (12)	0.0292 (13)	0.0204 (12)	0.0067 (9)	0.0055 (9)	0.0094 (10)
C20	0.0234 (12)	0.0248 (12)	0.0281 (13)	0.0047 (9)	0.0084 (10)	0.0095 (11)
C21	0.0428 (16)	0.0438 (16)	0.0281 (14)	0.0121 (12)	0.0126 (12)	0.0062 (12)
C22	0.0233 (13)	0.0302 (14)	0.0507 (17)	0.0067 (10)	0.0119 (11)	0.0171 (12)
C23	0.0316 (14)	0.0253 (13)	0.0554 (18)	0.0097 (10)	0.0209 (12)	0.0158 (12)
C24	0.0289 (13)	0.0304 (13)	0.0261 (13)	0.0063 (10)	0.0078 (10)	0.0159 (11)
C25	0.0389 (14)	0.0332 (14)	0.0387 (15)	0.0097 (11)	0.0143 (12)	0.0229 (12)
C26	0.0602 (18)	0.0389 (15)	0.0285 (15)	0.0095 (13)	0.0167 (13)	0.0190 (12)
C27	0.0319 (14)	0.0413 (15)	0.0540 (18)	0.0082 (11)	0.0143 (12)	0.0284 (14)

Table S6. X-ray diffraction geometric parameters (Å, º)

O1—C15	1.373 (2)	C13—H13A	0.9900
O1—H1	0.948 (10)	C13—H13B	0.9900
N1—C1	1.458 (3)	C14—C19	1.390 (3)
N1—C2	1.470 (3)	C14—C15	1.401 (3)
N1—C6	1.475 (3)	C15—C16	1.402 (3)
N2—C5	1.461 (3)	C16—C17	1.399 (3)
N2—C13	1.468 (3)	C16—C20	1.538 (3)
N2—C4	1.472 (3)	C17—C18	1.390 (3)
C1—C5i	1.528 (3)	C17—H17	0.9500
C1—H1A	0.9900	C18—C19	1.389 (3)
C1—H1B	0.9900	C18—C24	1.535 (3)
C2—C3	1.515 (3)	C19—H19	0.9500
C2—H2A	0.9900	C20—C21	1.530 (3)
C2—H2B	0.9900	C20—C23	1.532 (3)
C3—C4	1.518 (3)	C20—C22	1.539 (3)
C3—H3A	0.9900	C21—H21A	0.9800
C3—H3B	0.9900	C21—H21B	0.9800
C4—H4A	0.9900	C21—H21C	0.9800
C4—H4B	0.9900	C22—H22A	0.9800
C5—C1i	1.528 (3)	C22—H22B	0.9800
C5—H5A	0.9900	C22—H22C	0.9800
C5—H5B	0.9900	C23—H23A	0.9800
C6—C7	1.509 (3)	C23—H23B	0.9800
C6—H6A	0.9900	C23—H23C	0.9800
C6—H6B	0.9900	C24—C25	1.527 (3)
C7—C8	1.384 (3)	C24—C26	1.528 (3)
C7—C12	1.390 (3)	C24—C27	1.532 (3)
C8—C9	1.390 (4)	C25—H25A	0.9800
C8—H8	0.9500	C25—H25B	0.9800
C9—C10	1.372 (4)	C25—H25C	0.9800
C9—H9	0.9500	C26—H26A	0.9800
C10—C11	1.381 (4)	C26—H26B	0.9800
C10—H10	0.9500	C26—H26C	0.9800
C11—C12	1.377 (3)	C27—H27A	0.9800
C11—H11	0.9500	C27—H27B	0.9800
C12—H12	0.9500	C27—H27C	0.9800
C13—C14	1.504 (3)		
C15—O1—H1	109 (2)	C19—C14—C15	118.94 (19)
C1—N1—C2	111.29 (17)	C19—C14—C13	121.16 (19)
C1—N1—C6	109.33 (18)	C15—C14—C13	119.90 (19)
C2—N1—C6	111.14 (17)	O1—C15—C14	119.82 (18)
C5—N2—C13	111.80 (17)	O1—C15—C16	118.79 (19)
C5—N2—C4	110.47 (16)	C14—C15—C16	121.38 (19)
C13—N2—C4	109.80 (16)	C17—C16—C15	116.53 (19)
N1—C1—C5i	113.93 (18)	C17—C16—C20	121.78 (18)
N1—C1—H1A	108.8	C15—C16—C20	121.68 (19)
C5i—C1—H1A	108.8	C18—C17—C16	124.07 (19)
N1—C1—H1B	108.8	C18—C17—H17	118.0

C5i—C1—H1B	108.8	C16—C17—H17	118.0
H1A—C1—H1B	107.7	C19—C18—C17	116.96 (19)
N1—C2—C3	113.72 (17)	C19—C18—C24	119.72 (19)
N1—C2—H2A	108.8	C17—C18—C24	123.31 (19)
C3—C2—H2A	108.8	C18—C19—C14	122.0 (2)
N1—C2—H2B	108.8	C18—C19—H19	119.0
C3—C2—H2B	108.8	C14—C19—H19	119.0
H2A—C2—H2B	107.7	C21—C20—C23	107.93 (19)
C2—C3—C4	112.01 (18)	C21—C20—C16	110.40 (17)
C2—C3—H3A	109.2	C23—C20—C16	111.97 (18)
C4—C3—H3A	109.2	C21—C20—C22	109.36 (19)
C2—C3—H3B	109.2	C23—C20—C22	107.66 (18)
C4—C3—H3B	109.2	C16—C20—C22	109.44 (18)
H3A—C3—H3B	107.9	C20—C21—H21A	109.5
N2—C4—C3	114.41 (17)	C20—C21—H21B	109.5
N2—C4—H4A	108.7	H21A—C21—H21B	109.5
C3—C4—H4A	108.7	C20—C21—H21C	109.5
N2—C4—H4B	108.7	H21A—C21—H21C	109.5
C3—C4—H4B	108.7	H21B—C21—H21C	109.5
H4A—C4—H4B	107.6	C20—C22—H22A	109.5
N2—C5—C1i	113.42 (17)	C20—C22—H22B	109.5
N2—C5—H5A	108.9	H22A—C22—H22B	109.5
C1i—C5—H5A	108.9	C20—C22—H22C	109.5
N2—C5—H5B	108.9	H22A—C22—H22C	109.5
C1i—C5—H5B	108.9	H22B—C22—H22C	109.5
H5A—C5—H5B	107.7	C20—C23—H23A	109.5
N1—C6—C7	113.07 (18)	C20—C23—H23B	109.5
N1—C6—H6A	109.0	H23A—C23—H23B	109.5
C7—C6—H6A	109.0	C20—C23—H23C	109.5
N1—C6—H6B	109.0	H23A—C23—H23C	109.5
C7—C6—H6B	109.0	H23B—C23—H23C	109.5
H6A—C6—H6B	107.8	C25—C24—C26	108.04 (19)
C8—C7—C12	118.1 (2)	C25—C24—C27	108.18 (19)
C8—C7—C6	122.2 (2)	C26—C24—C27	109.1 (2)
C12—C7—C6	119.6 (2)	C25—C24—C18	112.55 (18)
C7—C8—C9	120.6 (2)	C26—C24—C18	110.63 (18)
C7—C8—H8	119.7	C27—C24—C18	108.27 (18)
C9—C8—H8	119.7	C24—C25—H25A	109.5
C10—C9—C8	120.7 (2)	C24—C25—H25B	109.5
C10—C9—H9	119.7	H25A—C25—H25B	109.5
C8—C9—H9	119.7	C24—C25—H25C	109.5
C9—C10—C11	119.1 (3)	H25A—C25—H25C	109.5
C9—C10—H10	120.4	H25B—C25—H25C	109.5
C11—C10—H10	120.4	C24—C26—H26A	109.5
C12—C11—C10	120.4 (3)	C24—C26—H26B	109.5
C12—C11—H11	119.8	H26A—C26—H26B	109.5
C10—C11—H11	119.8	C24—C26—H26C	109.5
C11—C12—C7	121.0 (2)	H26A—C26—H26C	109.5
C11—C12—H12	119.5	H26B—C26—H26C	109.5
C7—C12—H12	119.5	C24—C27—H27A	109.5

N2—C13—C14	112.16 (17)	C24—C27—H27B	109.5
N2—C13—H13A	109.2	H27A—C27—H27B	109.5
C14—C13—H13A	109.2	C24—C27—H27C	109.5
N2—C13—H13B	109.2	H27A—C27—H27C	109.5
C14—C13—H13B	109.2	H27B—C27—H27C	109.5
H13A—C13—H13B	107.9		
C2—N1—C1—C5i	67.0 (2)	C13—C14—C15—O1	2.3 (3)
C6—N1—C1—C5i	−169.87 (18)	C19—C14—C15—C16	3.4 (3)
C1—N1—C2—C3	−167.78 (18)	C13—C14—C15—C16	−176.55 (19)
C6—N1—C2—C3	70.1 (2)	O1—C15—C16—C17	178.37 (18)
N1—C2—C3—C4	172.83 (17)	C14—C15—C16—C17	−2.8 (3)
C5—N2—C4—C3	−75.3 (2)	O1—C15—C16—C20	−3.1 (3)
C13—N2—C4—C3	160.93 (17)	C14—C15—C16—C20	175.7 (2)
C2—C3—C4—N2	−66.7 (2)	C15—C16—C17—C18	0.0 (3)
C13—N2—C5—C1i	−64.3 (2)	C20—C16—C17—C18	−178.5 (2)
C4—N2—C5—C1i	173.11 (17)	C16—C17—C18—C19	2.1 (3)
C1—N1—C6—C7	70.1 (2)	C16—C17—C18—C24	−176.8 (2)
C2—N1—C6—C7	−166.69 (18)	C17—C18—C19—C14	−1.5 (3)
N1—C6—C7—C8	−118.2 (2)	C24—C18—C19—C14	177.40 (19)
N1—C6—C7—C12	63.2 (3)	C15—C14—C19—C18	−1.1 (3)
C12—C7—C8—C9	1.4 (3)	C13—C14—C19—C18	178.80 (19)
C6—C7—C8—C9	−177.2 (2)	C17—C16—C20—C21	−118.4 (2)
C7—C8—C9—C10	−0.3 (4)	C15—C16—C20—C21	63.2 (3)
C8—C9—C10—C11	−0.3 (4)	C17—C16—C20—C23	1.9 (3)
C9—C10—C11—C12	−0.2 (4)	C15—C16—C20—C23	−176.6 (2)
C10—C11—C12—C7	1.3 (4)	C17—C16—C20—C22	121.2 (2)
C8—C7—C12—C11	−2.0 (3)	C15—C16—C20—C22	−57.3 (3)
C6—C7—C12—C11	176.7 (2)	C19—C18—C24—C25	175.2 (2)
C5—N2—C13—C14	168.17 (17)	C17—C18—C24—C25	−6.0 (3)
C4—N2—C13—C14	−68.8 (2)	C19—C18—C24—C26	54.2 (3)
N2—C13—C14—C19	122.9 (2)	C17—C18—C24—C26	−127.0 (2)
N2—C13—C14—C15	−57.2 (3)	C19—C18—C24—C27	−65.3 (3)
C19—C14—C15—O1	−177.83 (19)	C17—C18—C24—C27	113.6 (2)

Symmetry code: (i) −x+2, −y+1, −z+1.

Table S7. Hydrogen-bond geometry (Å,°) for compound **4**

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N2	0.95 (1)	2.08 (2)	2.869 (2)	139 (3)
O1—H1···N1^{i}	0.95 (1)	2.28 (2)	3.055 (2)	138 (3)

Symmetry code: (i) −x+2, −y+1, −z+1.