Electronic Supplementary Information (ESI) for Dalton Transaction

Accompanying the manuscript

Dinuclear and 1D iron(III) Schiff base complexes bridged by 4-salicylideneamino-1,2,4-triazolate: X-ray structures and magnetic properties.

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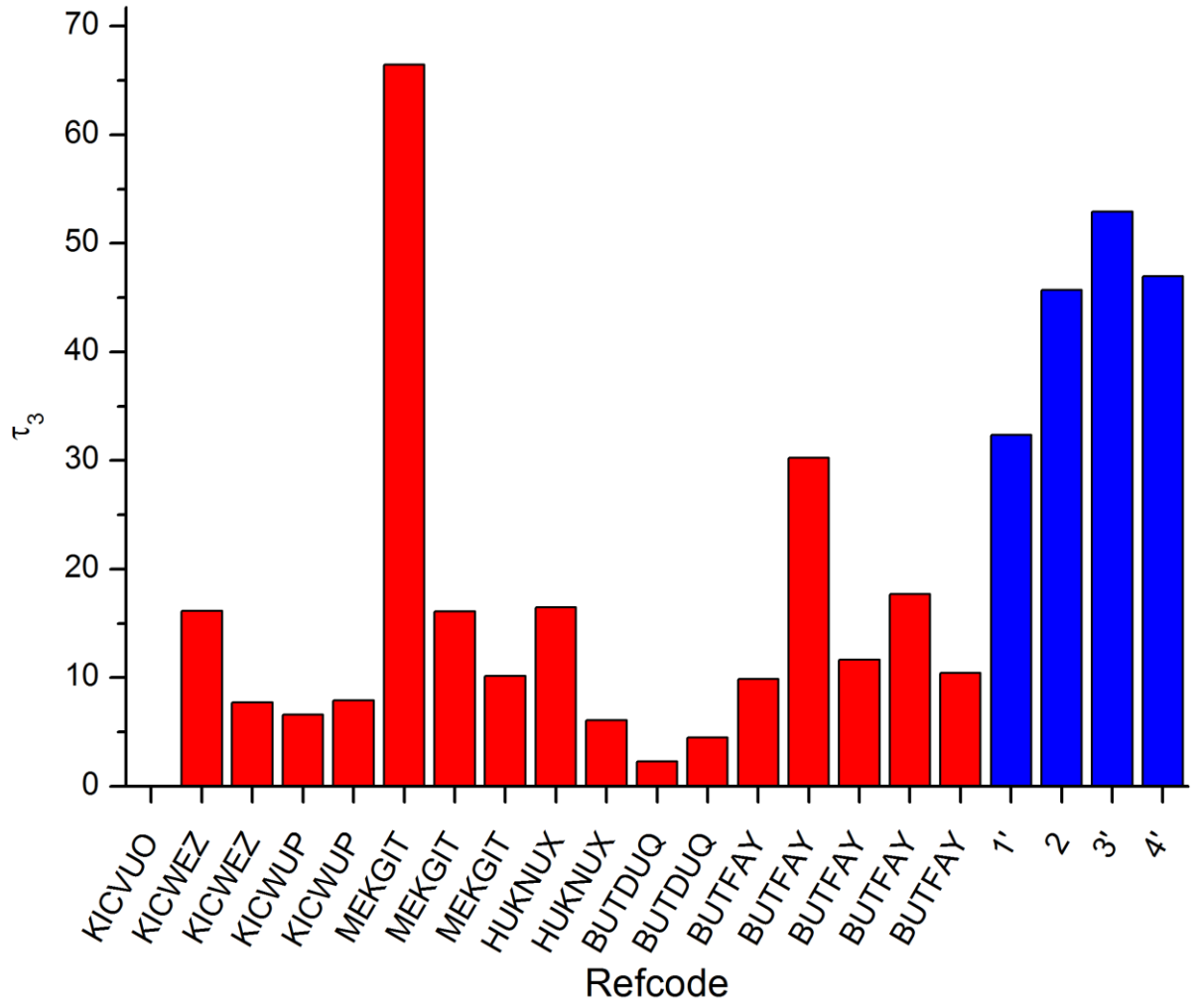

Fig. S1 Variation of τ_3 parameter in Hsaltrz and saltrz anion according to Cambridge Crystalligraphic Database (CSD). τ_3 is defined as dihedral angle between the least-squares benzene and triazole planes of Hsaltrz/saltrz.

KICVUO	$[Ag_2(\mu\text{-Hsaltrz})_2(CH_3CN)_2](ClO_4)_2$
KICWEZ	$[Ag_2(\mu\text{-Hsaltrz})_2(Hsaltrz)_2](BF_4)_2{\cdot}2H_2O$,
KICWUP	$[Ag_2(\mu\text{-Hsaltrz})_2\,(Hsaltrz)_2](NO_3)_2$
MEKGIT	$[Ag_4(\mu\text{-Hsaltrz})_6(CH_3CN)_2](AsF_6)_4{\cdot}2H_2O$
HUKNUX	Hsaltrz
BUTDUQ	$[Zn(Hsaltrz)_2(SCN)_2]$
BUTFAY	$[Co_2(\mu\text{-Hsaltrz})_3(Hsaltrz)_2(SCN)_4]{\cdot}H_2O$
1’	$[\{Fe(salen)(\mu\text{-saltrz})\}_2]{\cdot}CH_3OH{\cdot}(H_2O)_{0.5}$
2	$[\{Fe(salpn)(\mu\text{-saltrz})\}_2]$
3’	$[\{Fe(salch)(\mu\text{-saltrz})\}{\cdot}CH_3OH]_n$
4’	$[\{Fe(salophen)(\mu\text{-saltrz})\}{\cdot}CH_3OH]_n$

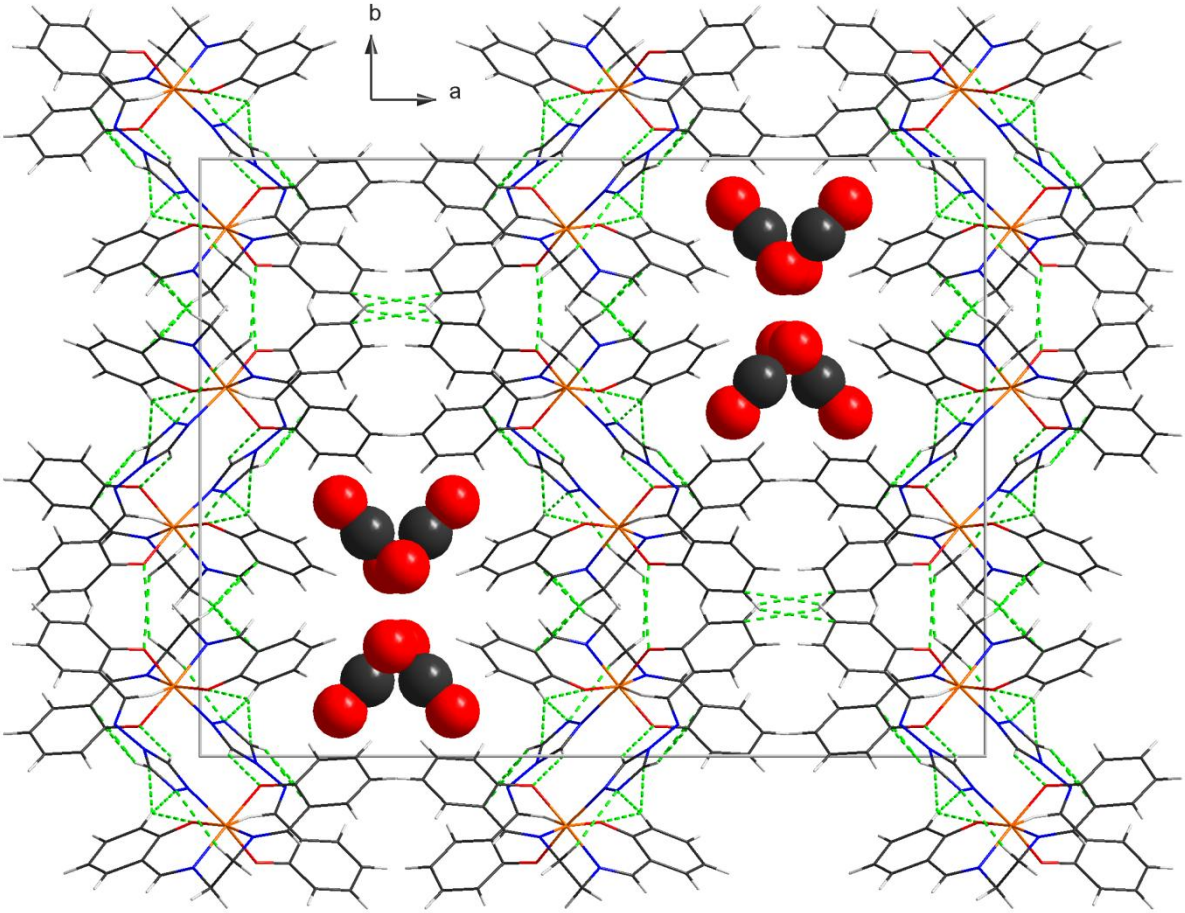

Fig. S2 Part of the crystal structure of [{Fe(salen)(μ-saltrz)}$_2$]·CH_3OH·$(H_2O)_{0.5}$ (**1'**), showing selected non-covalent contacts (dashed lines) and the cavities filled by solvent molecules, which are visualized using the space-filling model. (Parameters are given in Table S1).

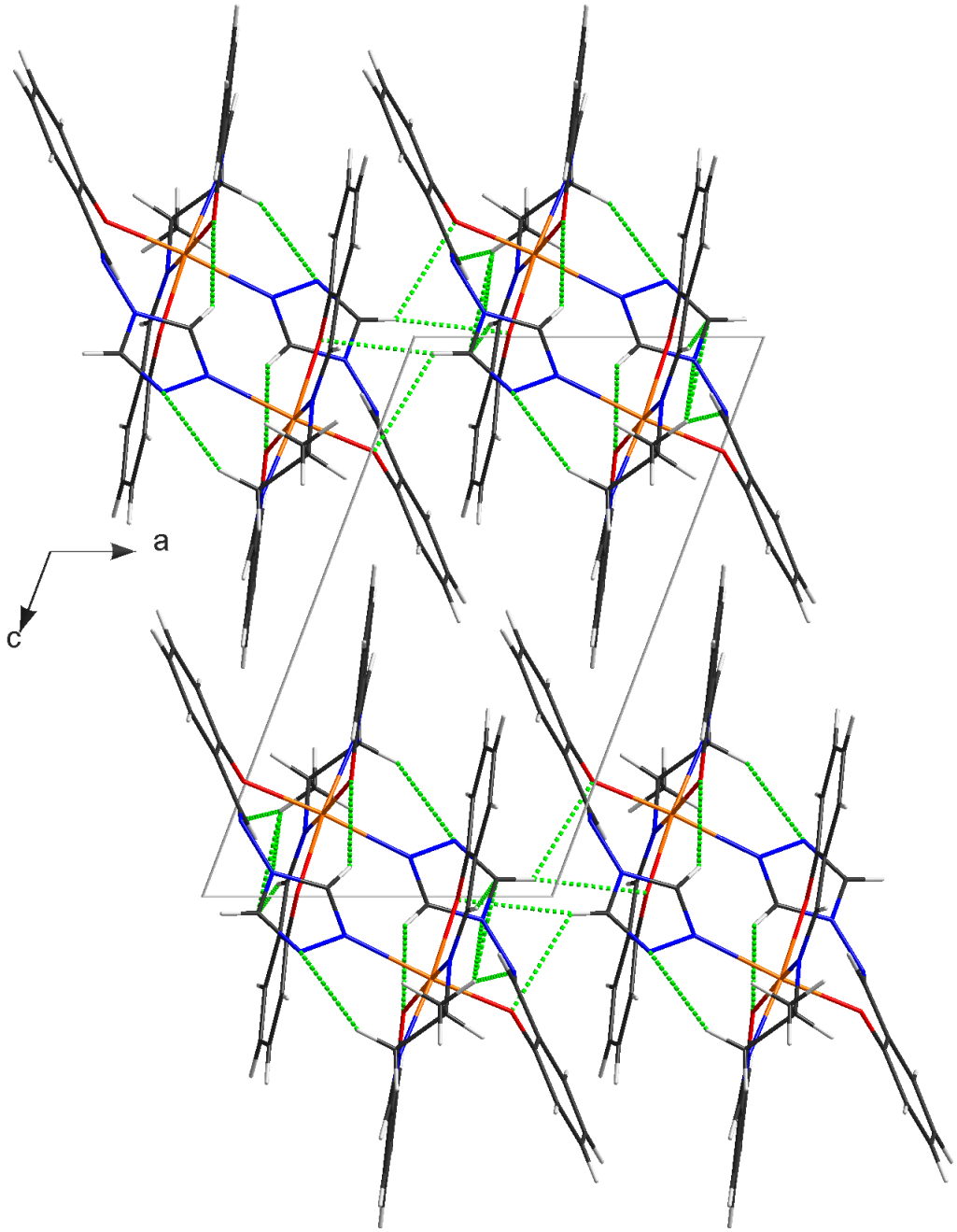

Fig. S3 Part of the crystal structure of [{Fe(salpn)(μ-saltrz)}$_2$] (**2**), showing selected non-covalent contacts (dashed lines) of the the C–H···C, C–H···N and C–H···O (Parameters are given in Table S1).

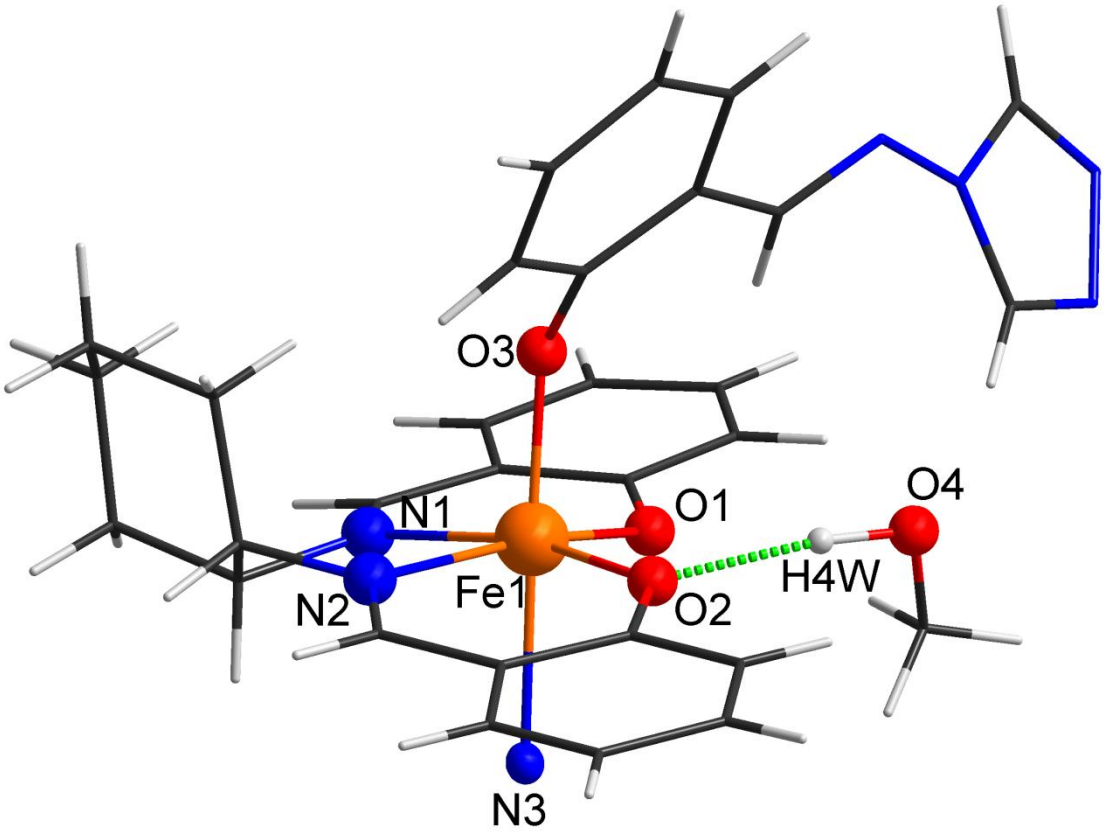

Fig. S4 The H-bond formation (dashed line) between methanol and the salch anion in X-ray structure of [{Fe(salch)(μ-saltrz)}·CH_3OH]$_n$ (**3**') (Parameters are given in Table S1).

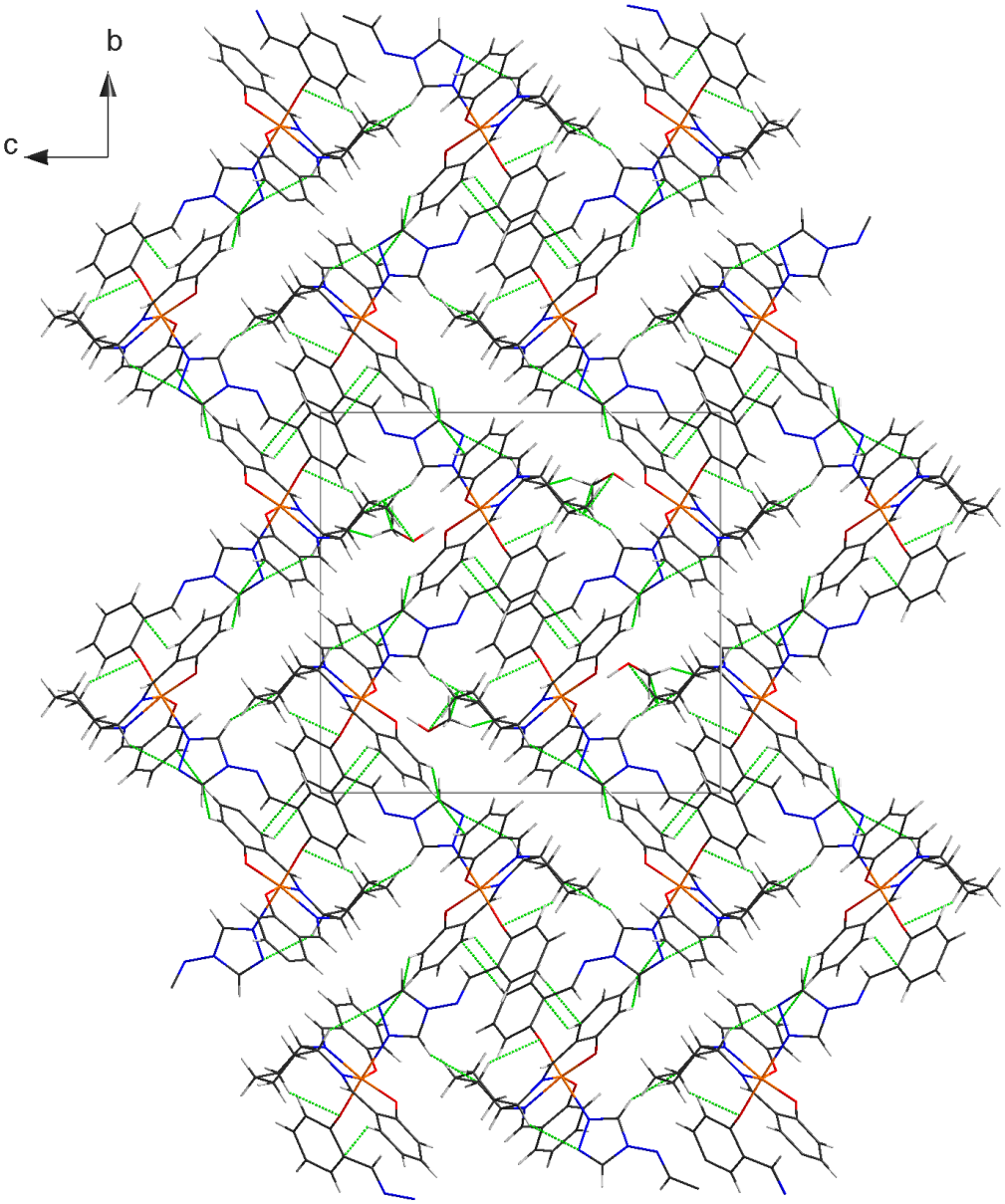

Fig. S5 Part of the crystal structure of [{Fe(salch)(μ-saltrz)}·CH_3OH]$_n$ (**3'**), showing selected non-covalent contacts (dashed lines) of the C–H···C and C–H···O types (Parameters are given in Table S1).

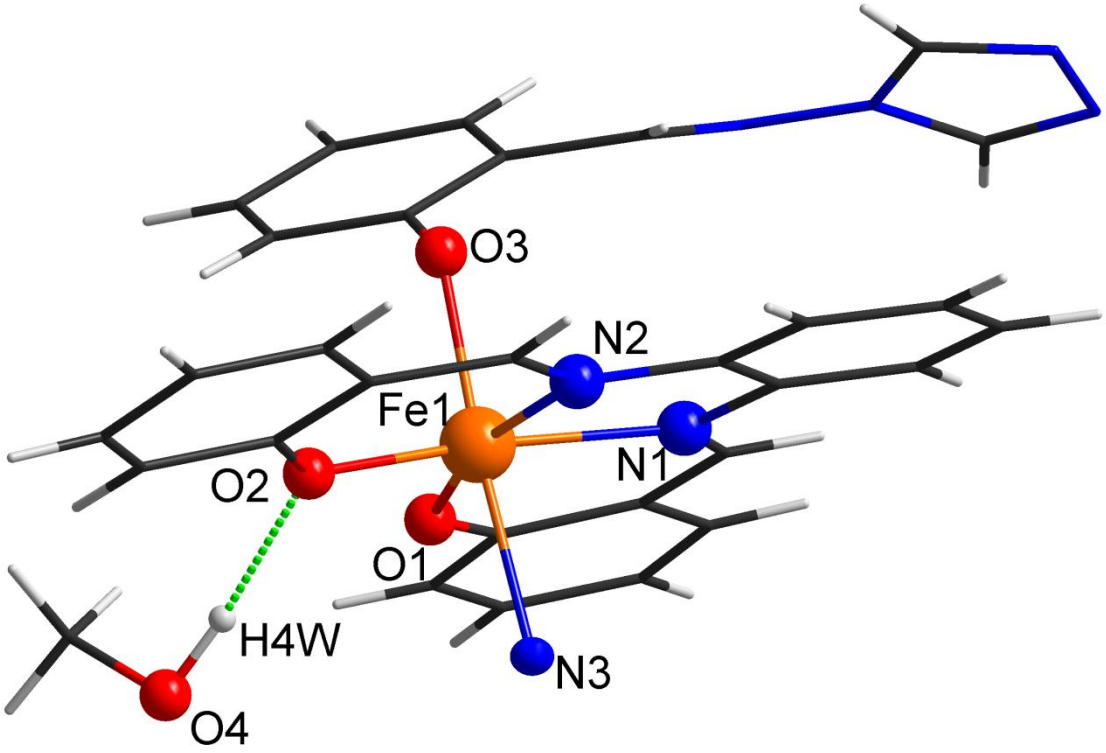

Fig. S6 The H-bond formation (dashed line) between methanol and salophen anion in X-ray structure of [{Fe(salophen)(μ-saltrz)}·CH_3OH]$_n$ (**4**') (Parameters are given in Table S1).

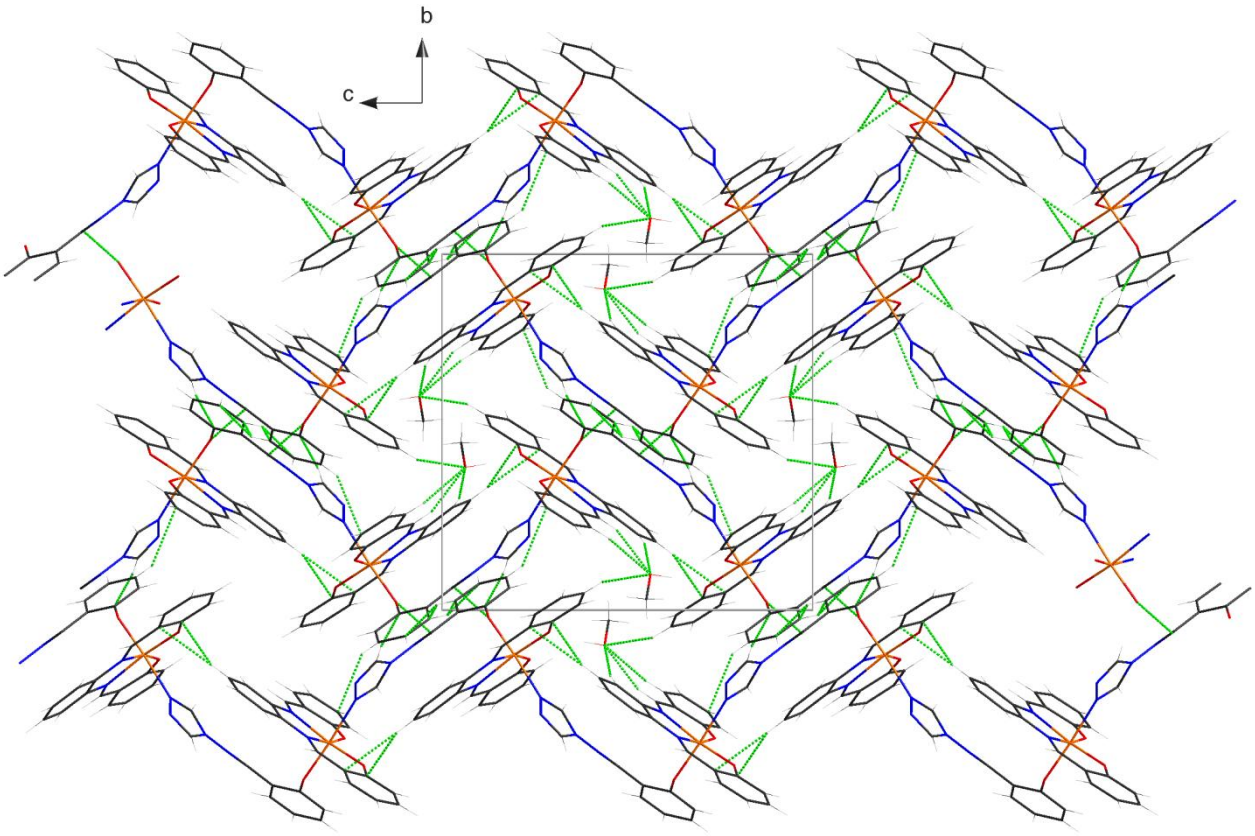

Fig. S7 Part of the crystal structure of [{Fe(salophen)(μ-saltrz)}·CH_3OH]$_n$ (**4**'), showing selected non-covalent contacts (dashed lines) of the C–H···C and C–H···O (Parameters are given in Table S1).

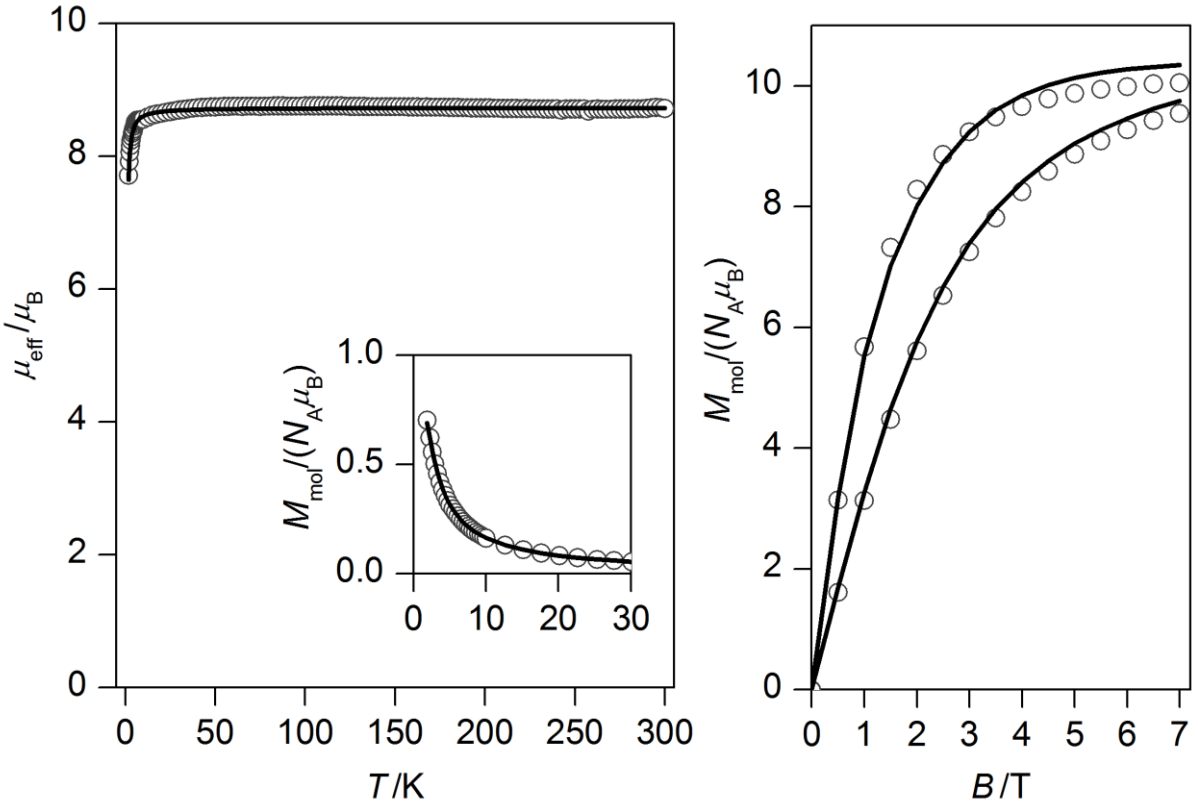

Fig. S8 Magnetic properties of **1**. Left: temperature dependence of effective magnetic moment (calculated from the temperature dependence of magnetization at B = 0.1 T; inset). Right: the isothermal magnetizations measured at T = 2.0 and 4.6 K. Experimental data - circles, full lines - the best fit calculated using equation 1 with: J = -0.063 cm^{-1}, g = 2.09 and D = -0.55 cm^{-1}.

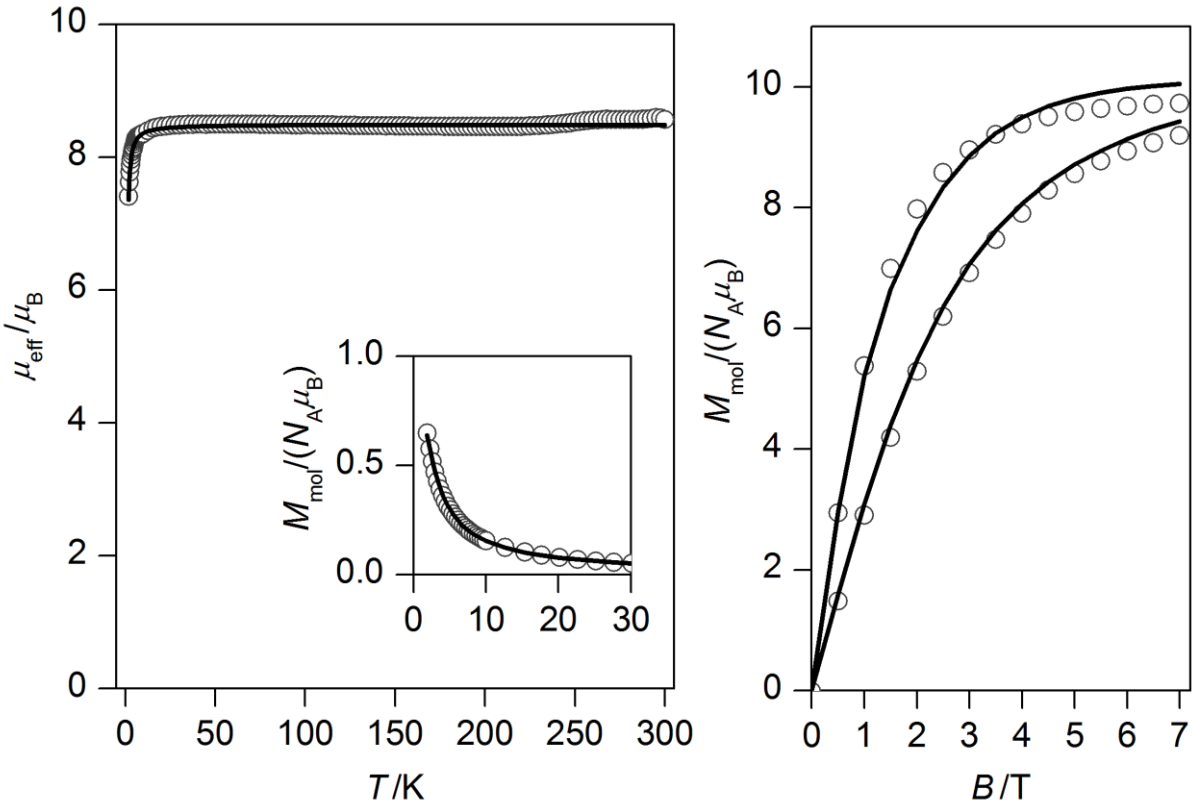

Fig. S9 Magnetic properties of **2**. Left: temperature dependence of effective magnetic moment (calculated from the temperature dependence of magnetization at B = 0.1 T; inset). Right: the isothermal magnetizations measured at T = 2.0 and 4.6 K. Experimental data - circles, full lines - the best fit calculated using equation 1with: J = -0.068 cm^{-1}, g = 2.03 and D = -0.58 cm^{-1}.

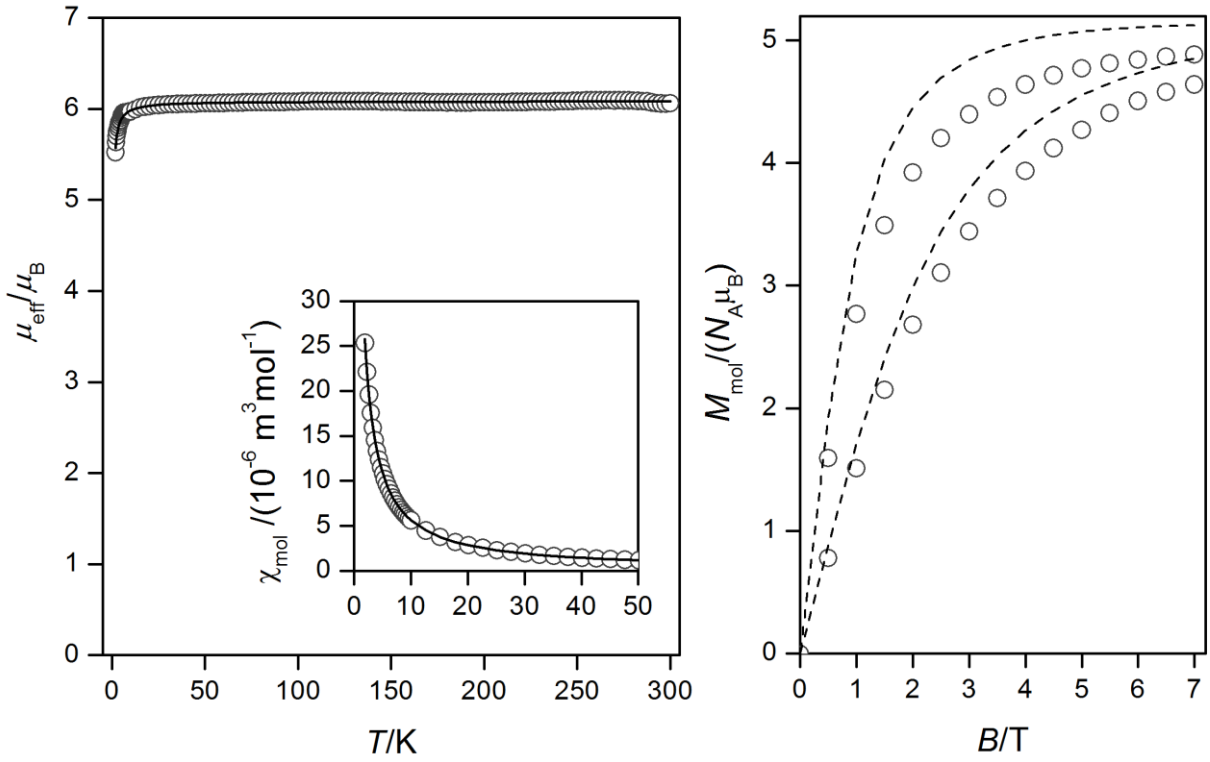

Fig. S10 Magnetic properties of **3** scaled per one Fe(III). Left: temperature dependence of effective magnetic moment (calculated from the temperature dependence of mean susceptibility at B = 0.1 T; inset). Right: the isothermal magnetizations measured at T = 2.0 and 4.6 K. Experimental data - circles, full lines - the best fit calculated using equation 3 with: J = -0.040 cm^{-1}, g = 2.06. Dotted line – theoretical magnetization calculated using Brillouin function for isolated S = 5/2.

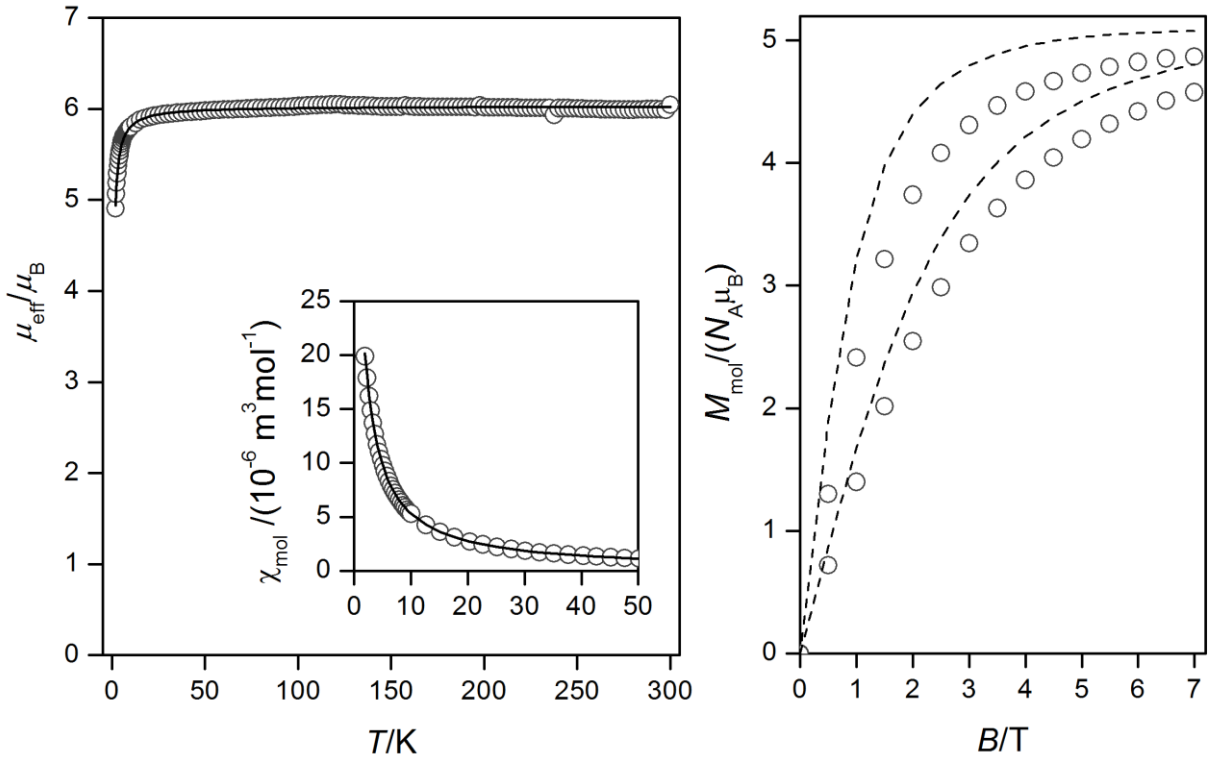

Fig. S11 Magnetic properties of **4** scaled per one Fe(III). Left: temperature dependence of effective magnetic moment (calculated from the temperature dependence of mean susceptibility at B = 0.1 T; inset). Right: the isothermal magnetizations measured at T = 2.0 and 4.6 K. Experimental data - circles, full lines - the best fit calculated using equation 3 with: J = -0.091 cm^{-1}, g = 2.04. Dotted line – theoretical magnetization calculated using Brillouin function for isolated S = 5/2.

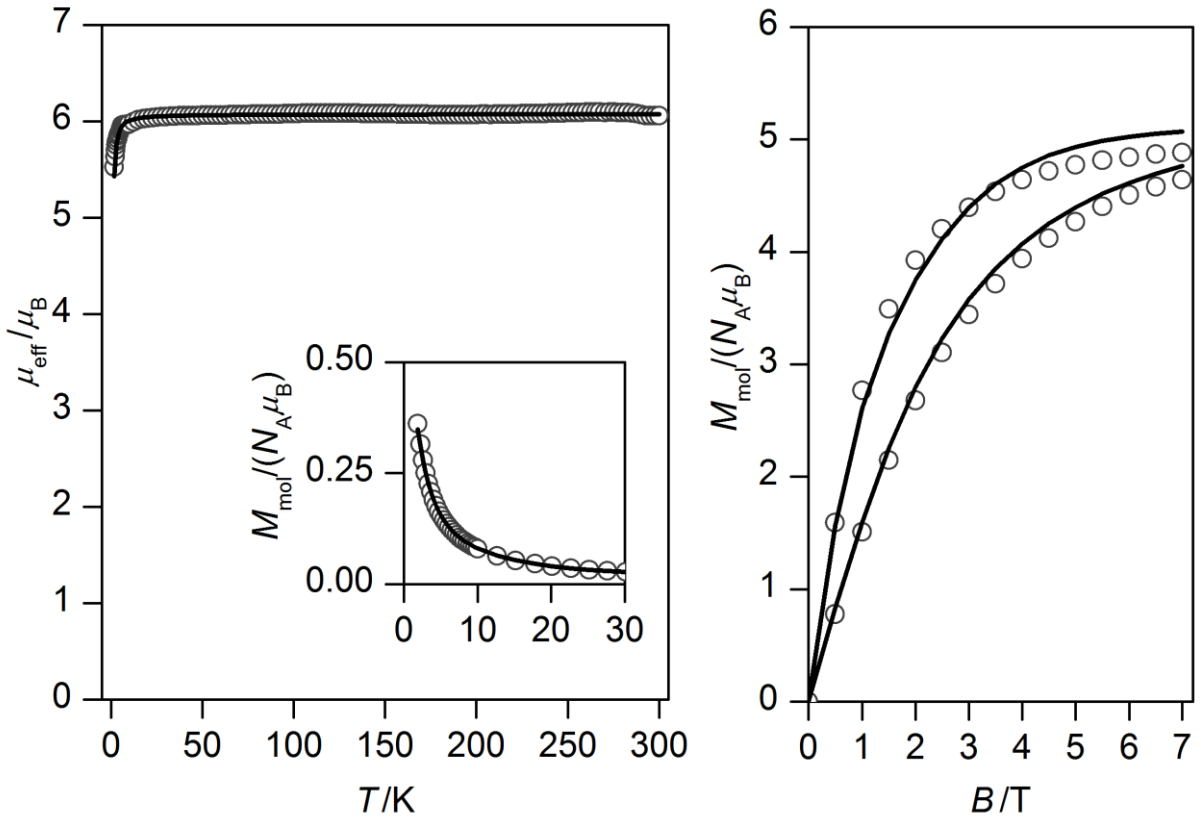

Fig. S12 Magnetic properties of **3** scaled per one Fe(III). Left: temperature dependence of effective magnetic moment (calculated from the temperature dependence of magnetization at B = 0.1 T; inset). Right: the isothermal magnetizations measured at T = 2.0 and 4.6 K. Experimental data - circles, full lines - the best fit calculated using equation 4 with: J = -0.022 cm^{-1}, g = 2.05 and D = -0.69 cm^{-1}.

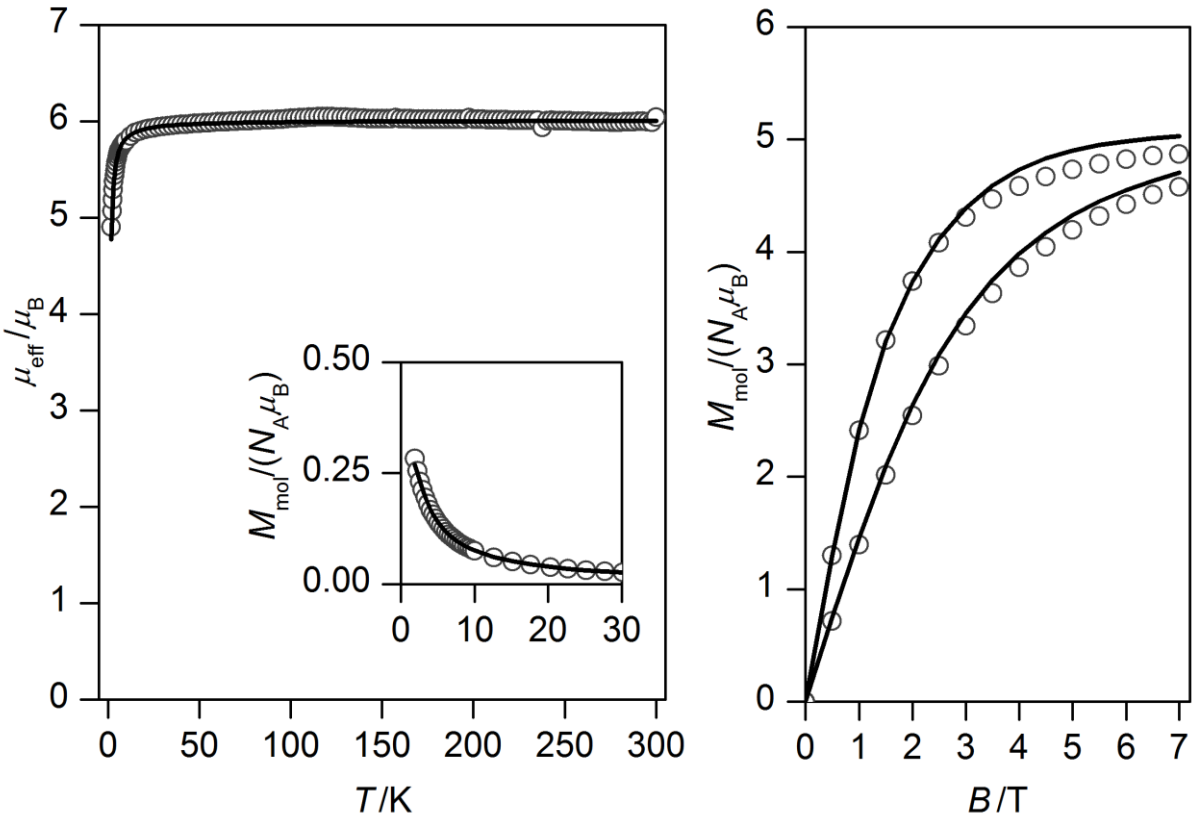

Fig. S13 Magnetic properties of **4** scaled per one Fe(III). Left: temperature dependence of effective magnetic moment (calculated from the temperature dependence of magnetization at B = 0.1 T; inset). Right: the isothermal magnetizations measured at T = 2.0 and 4.6 K. Experimental data - circles, full lines - the best fit calculated using equation 4 with: J = -0.072 cm^{-1}, g = 2.03 and D = -0.54 cm^{-1}.

Table S1 Hydrogen bonds and non-covalent contacts for **1'**–**4**'

	D–H...A	*d*(D–H)/Å	*d*(H...A)/Å	*d*(D...A)/Å	<(DHA)/°
1'	C18–H18A...C16[a]	0.9496(42)	2.8846(37)	3.6445(55)	137.819(262)
	C18–H18A...C11[a]	0.9496(42)	2.756(4)	3.6661(58)	160.825(265)
	C17...N6[a]			3.0106(51)	
	C22–H22A...C22[b]	0.9488(38)	2.8033(37)	3.5230(53)	133.370(237)
	C9–H9A...O3[c]	0.9888(39)	2.7043(24)	3.3328(46)	121.777(232)
	C8–H8A...C7[c]	0.9897(40)	2.7316(40)	3.6781(57)	160.201(248)
	C8–H8A...C6[c]	0.9897(40)	2.7545(37)	3.7020(54)	160.464(244)
	C8...O3[d]			3.0640(46)	
	C2–H2A...C18[e]	0.9492(40)	2.8849(41)	3.7487(58)	151.862(258)
	C2–H2A...N4[e]	0.9492(40)	2.7253(33)	3.6243(53)	158.308(256)
2	C16–H16A...C8[f]	0.9497(36)	2.7858(36)	3.7221(52)	168.879(225)
	C19–H19A...C8[f]	0.9797(65)	2.7414(31)	3.5462(67)	139.765(302)
	C19–H19A...N5[f]	0.9797(65)	2.7247(27)	3.4115(62)	127.568(289)
	C8...C7[g]			3.1797(47)	
	C8–H8A...C10[g]	0.9494(36)	2.8597(31)	3.7121(47)	149.962(215)
	C8–H8A...O1[g]	0.9494(36)	2.5992(24)	3.4687(42)	152.441(217)
	C8–H8A...O3[g]	0.9494(36)	2.6348(25)	3.2452(43)	122.499(189)
3'	O4–H4W...O2	1.0430(18)	1.8395(14)	2.8749(23)	171.286(111)
	C21–H21A...C30[h]	0.9900(18)	2.7208(28)	3.4919(33)	135.019(132)
	C21–H21A...O4[h]	0.9900(18)	2.6470(17)	3.3916(26)	132.143(128)
	C14–H14A...C5[i]	0.9506(18)	2.8585(20)	3.4863(27)	124.525(134)
	C12–H12A...C27[j]	0.9499(24)	2.8290(22)	3.6003(35)	139.003(152)
	C9–H9A...C19[k]	0.9495(21)	2.8420(23)	3.5864(33)	136.028(137)
	C4–H4A...C14[l]	0.9501(23)	2.7526(23)	3.6568(33)	159.303(136)
	C30–H30A...C22[m]	0.9802(28)	2.8627(18)	3.4645(31)	120.488(176)
	C8–H8A...C30	0.9498(21)	2.5929(29)	3.4996(36)	159.777(143)
	C8–H8A...O4	0.9498(21)	2.2416(19)	3.1706(28)	165.693(135)
	C30–H30C...O1	0.9793(28)	2.3500(13)	3.0596(28)	128.723(174)
	O4–H4W...C29	1.0430(18)	2.7923(20)	3.7764(27)	157.359(109)
4'	O4–H4W...O2	0.9581(15)	1.8244(13)	2.7690(19)	168.088(107)
	C12–H12A...C23[n]	0.9501(25)	2.8400(21)	3.4050(32)	119.116(145)
	C12–H12A...O4[o]	0.9501(25)	2.7006(18)	3.5319(32)	146.490(146)
	C3–H3A...C27[p]	0.9498(21)	2.8167(25)	3.4839(34)	128.102(145)
	C5...C18[q]			3.3404(30)	
	C5–H5A...C4[r]	0.9501(26)	2.8308(25)	3.6890(36)	150.738(147)
	C5–H5A...C5[r]	0.9501(26)	2.7618(24)	3.4558(36)	130.564(148)
	C7...C16[q]			3.3132(30)	
	C10...C9[q]			3.3489(32)	
	C9–H9A...C1[q]	0.9504(24)	2.8033(24)	3.7347(34)	166.702(146)
	C9–H9A...O3[q]	0.9504(24)	2.2587(15)	3.1833(28)	164.076(142)
	C20–H20A...C10[s]	0.9491(24)	2.8535(24)	3.6402(34)	140.976(147)
	C20–H20A...C15[s]	0.9491(24)	2.8436(22)	3.7769(33)	167.911(147)
	C23–H23A...O4[s]	0.9494(22)	2.5200(17)	3.4141(29)	156.995(137)
	C29–H29A...O4[s]	0.9493(24)	2.6863(15)	3.5344(27)	149.055(148)
	O4–H4W...C10	0.9581(15)	2.717(2)	3.5287(25)	142.879(109)

Symmetry transformations used to generate equivalent atoms:

[a] #1 1-x, 1-, -z #2 x, y, 1+z.
[b] #1 3/2-x, 1/2-y, z #2 x-1/2, y+1/2, 1-z.
[c] #1 x, 1/2-y, z-1/2 #2 1-x, 1/2-y, z+1/2.
[d] #1 x, 1/2-y, z+1/2 #2 1-x, 1/2+y, 1/2-z.
[e] #1 x, y, 1+z #2 1-x, 1-y, -z.
[f] #1 x, y-1,z #2 1-x, 2-y, -z.
[g] #1 -x, 1-y,-z #2 1+x, y, z.
[h] x-1, 3/2-y, z-1/2.
[i] 1+x, y, z.
[j] 1-x, y-1/2, 3/2-z.
[k] x, 3/2-y, 1/2+z.
[l] 1-x, 1-y, 1-z.
[m] 1+x, 3/2-y, 1/2+z.
[n] 1-x, y-1/2, 1/2-z.
[o] 1-x, 1-y, -z.
[p] -x, y-1/2, 1/2-z.
[q] 1-x, 1-y, 1-z.
[r] -x, 1-y, 1-z.
[s] x, 3/2-y, z+1/2