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Crystal structures and Hirshfeld surface analyses of (*E*)-*N*′-benzylidene-2-oxo-2*H*-chromene-3-carbohydrazide and the disordered hemi-DMSO solvate of (*E*)-2-oxo-*N*′-(3,4,5-trimethoxybenzylidene)-2*H*-chromene-3-carbohydrazide: lattice energy and intermolecular interaction energy calculations for the former. Corrigendum

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In the paper by Gomes *et al.* [*Acta Cryst.* (2019), E**75**, 1403–1410], there was an error and omission in the author and affiliation list.

In the paper by Gomes *et al.* (2019), one author was omitted (*i.e.* José Daniel Figueroa Villar) and the name and affiliations of another author (*i.e.*Camila Capelini) have been corrected. The complete and correct author list is given above.

References

Gomes, L. R., Low, J. N., Wardell, J. L., Capelini, C., Câmara, V. R. F., da Silva, E. F. & Carvalho, S. A. (2019). *Acta Cryst.* E**75**, 1403–1410.

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Crystal structures and Hirshfeld surface analyses of (*E*)-*N*′-benzylidene-2-oxo-2*H*-chromene-3-carbohydrazide and the disordered hemi-DMSO solvate of (*E*)-2-oxo-*N*′-(3,4,5-trimethoxybenzylidene)-2*H*-chromene-3-carbohydrazide: lattice energy and intermolecular interaction energy calculations for the former. Corrigendum

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(*E*)-2-Oxo-*N*′-(3,4,5-trimethoxybenzylidene)-2*H*-chromene-3-carbohydrazide dimethyl sulfoxide hemisolvate (I)

Crystal data

$C_{20}H_{18}N_2O_6·0.5C_2H_6OS$
M_r = 421.43
Monoclinic, *C*2/*c*
a = 33.0258 (7) Å
b = 5.4412 (1) Å
c = 22.4342 (4) Å
β = 107.203 (2)°
V = 3851.07 (13) Å^3
Z = 8
F(000) = 1768
D_x = 1.454 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71075 Å
Cell parameters from 13857 reflections
θ = 2.0–31.6°
μ = 0.16 mm^{-1}
T = 100 K
Block, yellow
0.40 × 0.08 × 0.04 mm

Data collection

Rigaku FRE+ equipped with VHF Varimax confocal mirrors and an AFC12 goniometer and HyPix 6000 detector diffractometer
Radiation source: Rotating Anode, Rigaku FRE+
Confocal mirrors, VHF Varimax monochromator
Detector resolution: 10 pixels mm^{-1}
profile data from *ω*–scans
Absorption correction: gaussian (CrysAlisPro; Rigaku OD, 2019)
T_{min} = 0.837, T_{max} = 1.000
22915 measured reflections
4381 independent reflections
3983 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
θ_{max} = 27.5°, θ_{min} = 2.6°
h = −42→42
k = −6→7
l = −26→29

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.086
S = 1.05
4381 reflections
298 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0456P)^2 + 2.9167P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ 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}	Occ. (<1)
O1	0.40457 (2)	0.68439 (13)	0.52398 (3)	0.01627 (16)	
O2	0.46021 (2)	0.81610 (14)	0.59671 (4)	0.02005 (17)	
O31	0.53178 (2)	0.20068 (14)	0.57120 (3)	0.01931 (17)	
O343	0.72470 (2)	0.31586 (14)	0.80720 (3)	0.01717 (16)	
O344	0.73938 (2)	0.64983 (14)	0.89856 (3)	0.01614 (16)	
O345	0.67832 (2)	0.95654 (15)	0.90901 (3)	0.02104 (17)	
N32	0.53224 (3)	0.55236 (18)	0.62643 (4)	0.01798 (19)	
H32	0.5171 (5)	0.679 (3)	0.6305 (7)	0.029 (4)*	
N33	0.57200 (3)	0.51012 (17)	0.66718 (4)	0.01668 (18)	
C2	0.44611 (3)	0.65614 (18)	0.55853 (4)	0.01415 (19)	
C3	0.46844 (3)	0.43809 (18)	0.54634 (4)	0.01325 (19)	
C4	0.44791 (3)	0.27552 (19)	0.50194 (4)	0.01369 (19)	
H4	0.462640	0.135045	0.494099	0.016*	
C5	0.38134 (3)	0.14563 (19)	0.42087 (5)	0.0175 (2)	
H5	0.394775	0.003909	0.410755	0.021*	
C4A	0.40442 (3)	0.31084 (18)	0.46651 (4)	0.01345 (19)	
C6	0.33896 (3)	0.1903 (2)	0.39072 (5)	0.0204 (2)	
H6	0.323245	0.077292	0.360352	0.024*	
C7	0.31911 (3)	0.4001 (2)	0.40457 (5)	0.0194 (2)	
H7	0.289997	0.428309	0.383493	0.023*	
C8	0.34135 (3)	0.5677 (2)	0.44868 (5)	0.0173 (2)	
H8	0.328020	0.711508	0.457860	0.021*	
C8A	0.38373 (3)	0.51893 (18)	0.47906 (4)	0.01401 (19)	
C31	0.51385 (3)	0.38442 (19)	0.58215 (4)	0.0144 (2)	
C34	0.58354 (3)	0.6722 (2)	0.70991 (5)	0.0234 (2)	
H34	0.565334	0.807515	0.709773	0.028*	
C341	0.62400 (3)	0.6560 (2)	0.75915 (5)	0.0182 (2)	
C342	0.65468 (3)	0.48341 (19)	0.75655 (4)	0.0154 (2)	
H342	0.649709	0.371929	0.722555	0.018*	
C343	0.69263 (3)	0.47723 (18)	0.80448 (4)	0.01379 (19)	
C344	0.70034 (3)	0.64402 (19)	0.85427 (4)	0.0140 (2)	
C345	0.66880 (3)	0.80974 (19)	0.85746 (5)	0.0165 (2)	
C346	0.63073 (3)	0.8169 (2)	0.80957 (5)	0.0207 (2)	
H346	0.609346	0.931306	0.811211	0.025*	
C431	0.71732 (4)	0.1389 (2)	0.75813 (5)	0.0207 (2)	
H43A	0.712251	0.223812	0.718061	0.031*	

H43B	0.692471	0.039486	0.757575	0.031*	
H43C	0.742175	0.032094	0.765084	0.031*	
C441	0.74230 (3)	0.4860 (2)	0.94982 (5)	0.0195 (2)	
H41A	0.736607	0.317514	0.934155	0.029*	
H41B	0.721429	0.533664	0.970960	0.029*	
H41C	0.770842	0.495051	0.979338	0.029*	
C451	0.64624 (3)	1.1251 (2)	0.91407 (5)	0.0196 (2)	
H51A	0.620280	1.034335	0.912316	0.029*	
H51B	0.640421	1.242953	0.879538	0.029*	
H51C	0.656046	1.213390	0.953827	0.029*	
S1S	0.50726 (2)	1.12167 (9)	0.72755 (2)	0.01665 (11)	0.5
O1S	0.4985 (16)	0.8678 (3)	0.7444 (12)	0.026 (2)	0.5
C1S	0.45886 (14)	1.2893 (14)	0.7013 (3)	0.0207 (9)	0.5
H1SA	0.442339	1.228493	0.660195	0.031*	0.5
H1SB	0.465103	1.464184	0.698321	0.031*	0.5
H1SC	0.442536	1.267478	0.730985	0.031*	0.5
C2S	0.52800 (15)	1.2784 (15)	0.7996 (3)	0.0300 (12)	0.5
H2SA	0.510606	1.241255	0.827053	0.045*	0.5
H2SB	0.527643	1.455833	0.791972	0.045*	0.5
H2SC	0.557203	1.224526	0.819443	0.045*	0.5

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0125 (3)	0.0167 (4)	0.0169 (3)	0.0020 (3)	0.0002 (3)	−0.0032 (3)
O2	0.0179 (4)	0.0181 (4)	0.0202 (4)	0.0021 (3)	−0.0004 (3)	−0.0066 (3)
O31	0.0143 (3)	0.0207 (4)	0.0198 (4)	0.0040 (3)	0.0002 (3)	−0.0052 (3)
O343	0.0150 (3)	0.0195 (4)	0.0151 (3)	0.0036 (3)	0.0015 (3)	−0.0017 (3)
O344	0.0122 (3)	0.0200 (4)	0.0129 (3)	−0.0033 (3)	−0.0014 (3)	0.0018 (3)
O345	0.0171 (4)	0.0253 (4)	0.0179 (4)	0.0004 (3)	0.0008 (3)	−0.0105 (3)
N32	0.0103 (4)	0.0222 (5)	0.0177 (4)	0.0040 (3)	−0.0017 (3)	−0.0063 (3)
N33	0.0104 (4)	0.0231 (5)	0.0144 (4)	0.0001 (3)	0.0003 (3)	−0.0022 (3)
C2	0.0122 (4)	0.0160 (5)	0.0130 (4)	0.0007 (4)	0.0018 (3)	0.0001 (4)
C3	0.0115 (4)	0.0149 (5)	0.0124 (4)	0.0008 (4)	0.0022 (3)	0.0002 (4)
C4	0.0135 (4)	0.0140 (5)	0.0130 (4)	0.0007 (4)	0.0031 (4)	0.0006 (4)
C5	0.0183 (5)	0.0165 (5)	0.0156 (5)	−0.0020 (4)	0.0018 (4)	−0.0006 (4)
C4A	0.0129 (4)	0.0147 (5)	0.0117 (4)	−0.0013 (4)	0.0021 (3)	0.0015 (3)
C6	0.0189 (5)	0.0223 (5)	0.0155 (5)	−0.0060 (4)	−0.0020 (4)	−0.0002 (4)
C7	0.0124 (5)	0.0248 (6)	0.0171 (5)	−0.0022 (4)	−0.0015 (4)	0.0060 (4)
C8	0.0139 (5)	0.0186 (5)	0.0183 (5)	0.0016 (4)	0.0031 (4)	0.0042 (4)
C8A	0.0135 (4)	0.0148 (5)	0.0125 (4)	−0.0021 (4)	0.0020 (4)	0.0008 (4)
C31	0.0119 (4)	0.0179 (5)	0.0123 (4)	0.0003 (4)	0.0019 (3)	−0.0009 (4)
C34	0.0143 (5)	0.0289 (6)	0.0226 (5)	0.0051 (4)	−0.0011 (4)	−0.0099 (4)
C341	0.0131 (5)	0.0229 (5)	0.0163 (5)	−0.0007 (4)	0.0008 (4)	−0.0050 (4)
C342	0.0142 (4)	0.0188 (5)	0.0122 (4)	−0.0016 (4)	0.0024 (4)	−0.0034 (4)
C343	0.0132 (4)	0.0151 (5)	0.0136 (4)	−0.0005 (4)	0.0047 (4)	0.0014 (4)
C344	0.0109 (4)	0.0177 (5)	0.0116 (4)	−0.0032 (4)	0.0007 (3)	0.0010 (4)
C345	0.0157 (5)	0.0191 (5)	0.0137 (5)	−0.0032 (4)	0.0031 (4)	−0.0049 (4)

C346	0.0140 (5)	0.0250 (6)	0.0209 (5)	0.0029 (4)	0.0019 (4)	−0.0081 (4)
C431	0.0224 (5)	0.0185 (5)	0.0203 (5)	0.0032 (4)	0.0051 (4)	−0.0037 (4)
C441	0.0193 (5)	0.0220 (5)	0.0145 (5)	−0.0009 (4)	0.0007 (4)	0.0032 (4)
C451	0.0180 (5)	0.0209 (5)	0.0205 (5)	−0.0021 (4)	0.0064 (4)	−0.0075 (4)
S1S	0.0182 (2)	0.0149 (2)	0.0183 (2)	0.00064 (18)	0.00770 (19)	−0.00093 (19)
O1S	0.040 (5)	0.0140 (6)	0.030 (7)	0.0000 (17)	0.020 (7)	−0.0005 (12)
C1S	0.019 (2)	0.0187 (14)	0.0218 (14)	0.003 (2)	0.0018 (17)	0.0027 (10)
C2S	0.033 (3)	0.024 (2)	0.0284 (17)	0.006 (3)	0.001 (2)	−0.0054 (13)

Geometric parameters (Å, º)

O1—C2	1.3702 (12)	C34—C341	1.4629 (14)
O1—C8A	1.3747 (12)	C34—H34	0.9500
O2—C2	1.2133 (12)	C341—C342	1.3953 (14)
O31—C31	1.2234 (13)	C341—C346	1.3955 (14)
O343—C343	1.3631 (12)	C342—C343	1.3894 (13)
O343—C431	1.4280 (12)	C342—H342	0.9500
O344—C344	1.3759 (11)	C343—C344	1.4028 (14)
O344—C441	1.4356 (12)	C344—C345	1.3955 (14)
O345—C345	1.3635 (12)	C345—C346	1.3921 (14)
O345—C451	1.4309 (13)	C346—H346	0.9500
N32—C31	1.3543 (13)	C431—H43A	0.9800
N32—N33	1.3793 (11)	C431—H43B	0.9800
N32—H32	0.870 (16)	C431—H43C	0.9800
N33—C34	1.2753 (14)	C441—H41A	0.9800
C2—C3	1.4647 (13)	C441—H41B	0.9800
C3—C4	1.3547 (14)	C441—H41C	0.9800
C3—C31	1.5056 (13)	C451—H51A	0.9800
C4—C4A	1.4340 (13)	C451—H51B	0.9800
C4—H4	0.9500	C451—H51C	0.9800
C5—C6	1.3840 (15)	S1S—O1S	1.483 (16)
C5—C4A	1.4057 (14)	S1S—C2S	1.775 (7)
C5—H5	0.9500	S1S—C1S	1.782 (5)
C4A—C8A	1.3935 (14)	C1S—H1SA	0.9800
C6—C7	1.3965 (16)	C1S—H1SB	0.9800
C6—H6	0.9500	C1S—H1SC	0.9800
C7—C8	1.3856 (15)	C2S—H2SA	0.9800
C7—H7	0.9500	C2S—H2SB	0.9800
C8—C8A	1.3890 (13)	C2S—H2SC	0.9800
C8—H8	0.9500		

C2—O1—C8A	122.80 (8)	C341—C342—H342	120.5
C343—O343—C431	116.52 (8)	O343—C343—C342	124.14 (9)
C344—O344—C441	113.00 (8)	O343—C343—C344	115.17 (8)
C345—O345—C451	116.90 (8)	C342—C343—C344	120.69 (9)
C31—N32—N33	120.41 (9)	O344—C344—C345	120.16 (9)
C31—N32—H32	117.6 (10)	O344—C344—C343	120.05 (9)
N33—N32—H32	121.7 (10)	C345—C344—C343	119.76 (9)

C34—N33—N32	113.41 (9)	O345—C345—C346	124.54 (9)
O2—C2—O1	115.46 (9)	O345—C345—C344	115.71 (9)
O2—C2—C3	127.12 (9)	C346—C345—C344	119.75 (9)
O1—C2—C3	117.42 (8)	C345—C346—C341	119.92 (10)
C4—C3—C2	119.74 (9)	C345—C346—H346	120.0
C4—C3—C31	117.95 (9)	C341—C346—H346	120.0
C2—C3—C31	122.31 (9)	O343—C431—H43A	109.5
C3—C4—C4A	121.44 (9)	O343—C431—H43B	109.5
C3—C4—H4	119.3	H43A—C431—H43B	109.5
C4A—C4—H4	119.3	O343—C431—H43C	109.5
C6—C5—C4A	119.72 (10)	H43A—C431—H43C	109.5
C6—C5—H5	120.1	H43B—C431—H43C	109.5
C4A—C5—H5	120.1	O344—C441—H41A	109.5
C8A—C4A—C5	118.30 (9)	O344—C441—H41B	109.5
C8A—C4A—C4	117.88 (9)	H41A—C441—H41B	109.5
C5—C4A—C4	123.81 (9)	O344—C441—H41C	109.5
C5—C6—C7	120.56 (10)	H41A—C441—H41C	109.5
C5—C6—H6	119.7	H41B—C441—H41C	109.5
C7—C6—H6	119.7	O345—C451—H51A	109.5
C8—C7—C6	120.80 (9)	O345—C451—H51B	109.5
C8—C7—H7	119.6	H51A—C451—H51B	109.5
C6—C7—H7	119.6	O345—C451—H51C	109.5
C7—C8—C8A	117.99 (10)	H51A—C451—H51C	109.5
C7—C8—H8	121.0	H51B—C451—H51C	109.5
C8A—C8—H8	121.0	O1S—S1S—C2S	105.5 (10)
O1—C8A—C8	116.63 (9)	O1S—S1S—C1S	109.8 (19)
O1—C8A—C4A	120.73 (9)	C2S—S1S—C1S	96.99 (18)
C8—C8A—C4A	122.62 (9)	S1S—C1S—H1SA	109.5
O31—C31—N32	124.05 (9)	S1S—C1S—H1SB	109.5
O31—C31—C3	121.09 (9)	H1SA—C1S—H1SB	109.5
N32—C31—C3	114.86 (9)	S1S—C1S—H1SC	109.5
N33—C34—C341	121.94 (10)	H1SA—C1S—H1SC	109.5
N33—C34—H34	119.0	H1SB—C1S—H1SC	109.5
C341—C34—H34	119.0	S1S—C2S—H2SA	109.5
C342—C341—C346	120.85 (9)	S1S—C2S—H2SB	109.5
C342—C341—C34	121.44 (9)	H2SA—C2S—H2SB	109.5
C346—C341—C34	117.71 (9)	S1S—C2S—H2SC	109.5
C343—C342—C341	118.94 (9)	H2SA—C2S—H2SC	109.5
C343—C342—H342	120.5	H2SB—C2S—H2SC	109.5

C31—N32—N33—C34	−173.67 (10)	C4—C3—C31—N32	−179.03 (9)
C8A—O1—C2—O2	−179.61 (9)	C2—C3—C31—N32	0.25 (14)
C8A—O1—C2—C3	−0.32 (13)	N32—N33—C34—C341	177.68 (10)
O2—C2—C3—C4	179.69 (10)	N33—C34—C341—C342	9.81 (18)
O1—C2—C3—C4	0.50 (14)	N33—C34—C341—C346	−169.23 (11)
O2—C2—C3—C31	0.42 (16)	C346—C341—C342—C343	−1.33 (16)
O1—C2—C3—C31	−178.77 (8)	C34—C341—C342—C343	179.66 (10)
C2—C3—C4—C4A	−0.40 (14)	C431—O343—C343—C342	−2.19 (14)

C31—C3—C4—C4A	178.90 (9)	C431—O343—C343—C344	178.22 (9)
C6—C5—C4A—C8A	−1.25 (15)	C341—C342—C343—O343	179.45 (9)
C6—C5—C4A—C4	177.48 (9)	C341—C342—C343—C344	−0.98 (15)
C3—C4—C4A—C8A	0.11 (14)	C441—O344—C344—C345	92.74 (11)
C3—C4—C4A—C5	−178.62 (9)	C441—O344—C344—C343	−89.56 (11)
C4A—C5—C6—C7	1.01 (16)	O343—C343—C344—O344	5.20 (13)
C5—C6—C7—C8	0.00 (16)	C342—C343—C344—O344	−174.41 (9)
C6—C7—C8—C8A	−0.72 (15)	O343—C343—C344—C345	−177.09 (9)
C2—O1—C8A—C8	178.49 (9)	C342—C343—C344—C345	3.30 (15)
C2—O1—C8A—C4A	0.04 (14)	C451—O345—C345—C346	1.34 (15)
C7—C8—C8A—O1	−177.96 (9)	C451—O345—C345—C344	−178.86 (9)
C7—C8—C8A—C4A	0.46 (15)	O344—C344—C345—O345	−5.41 (14)
C5—C4A—C8A—O1	178.88 (9)	C343—C344—C345—O345	176.88 (9)
C4—C4A—C8A—O1	0.08 (14)	O344—C344—C345—C346	174.40 (9)
C5—C4A—C8A—C8	0.52 (15)	C343—C344—C345—C346	−3.31 (15)
C4—C4A—C8A—C8	−178.28 (9)	O345—C345—C346—C341	−179.17 (10)
N33—N32—C31—O31	−7.04 (16)	C344—C345—C346—C341	1.03 (17)
N33—N32—C31—C3	172.52 (8)	C342—C341—C346—C345	1.31 (17)
C4—C3—C31—O31	0.54 (14)	C34—C341—C346—C345	−179.64 (10)
C2—C3—C31—O31	179.82 (9)		

Hydrogen-bond geometry (Å, º)

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the O1/C2–C4/C4*A*/C8*A*, C4*A*/C5–C8/C8*A* and C341–C346 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N32—H32···O2	0.870 (16)	1.955 (15)	2.6878 (12)	141.0 (14)
C441—H41*C*···O345^{i}	0.98	2.58	3.4772 (12)	152
C451—H51*A*···O1^{ii}	0.98	2.65	3.4463 (13)	138
C34—H34···O1*S*	0.95	2.57	3.30 (5)	134
C34—H34···O1*S*^{ii}	0.95	2.63	3.34 (5)	133
C34—H34···S1*S*	0.95	2.69	3.6158 (12)	166
C431—H43*C*···O343^{iii}	0.98	2.50	3.2505 (13)	133
C2*S*—H2*SA*···N32^{iv}	0.98	2.61	3.3000 (6)	127
C4—H4···O31	0.95	2.45	2.7761 (12)	100
C4—H4···O31^{v}	0.95	2.38	3.2415 (12)	150
C5—H5···O31^{v}	0.95	2.59	3.3931 (13)	143
C431—H43*B*···*Cg*3^{vi}	0.98	2.73	3.5882 (13)	147
C451—H51*B*···*Cg*3^{vi}	0.98	2.95	3.8562 (12)	155
C451—H51*C*···*Cg*2^{vii}	0.98	2.83	3.6883 (13)	147
C31—O31···*Cg*1^{vii}	0	0	3.3971 (6)	90 (1)

Symmetry codes: (i) −*x*+3/2, −*y*+3/2, −*z*+2; (ii) −*x*+1, *y*, −*z*+3/2; (iii) −*x*+3/2, *y*−1/2, −*z*+3/2; (iv) −*x*+1, *y*+1, −*z*+3/2; (v) −*x*+1, −*y*, −*z*+1; (vi) *x*, *y*−1, *z*; (vii) −*x*+1, −*y*+1, −*z*+1.

(*E*)-*N*′-Benzylidene-2-oxo-2*H*-chromene-3-carbohydrazide (II)

Crystal data

$C_{17}H_{12}N_2O_3$	Triclinic, $P\overline{1}$
M_r = 292.29	*a* = 5.6715 (1) Å

b = 7.4164 (1) Å
c = 15.9819 (3) Å
α = 88.369 (1)°
β = 84.147 (1)°
γ = 82.961 (2)°
V = 663.60 (2) Å^3
Z = 2
$F(000)$ = 304

D_x = 1.463 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 8290 reflections
θ = 6.0–70.3°
μ = 0.84 mm^{-1}
T = 100 K
Plate, colourless
0.22 × 0.12 × 0.05 mm

Data collection

Rigaku 007HF equipped with Varimax confocal mirrors and an AFC11 goniometer and HyPix 6000 detector diffractometer
Radiation source: Rotating anode, Rigaku 007 HF
Varimax focusing mirrors monochromator
Detector resolution: 10 pixels mm^{-1}
profile data from ω–scans

Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2019)
T_{min} = 0.930, T_{max} = 1.000
11641 measured reflections
2352 independent reflections
2250 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 67.1°, θ_{min} = 5.6°
h = −6→6
k = −8→8
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.104
S = 0.88
2352 reflections
203 parameters
0 restraints

Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0858P)^2 + 0.127P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 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}
O1	0.38486 (11)	0.36429 (9)	0.68964 (4)	0.0233 (2)
H1	0.276 (3)	0.3194 (18)	0.4545 (9)	0.043 (4)*
O2	0.19764 (11)	0.41255 (9)	0.57568 (4)	0.0256 (2)
O31	0.77445 (12)	0.11739 (10)	0.43121 (4)	0.0316 (2)
N32	0.40134 (15)	0.26503 (11)	0.42751 (5)	0.0220 (2)
N33	0.40966 (14)	0.23814 (10)	0.34233 (5)	0.0227 (2)
C2	0.37588 (16)	0.34215 (12)	0.60485 (6)	0.0213 (2)
C3	0.58217 (17)	0.23662 (12)	0.55958 (6)	0.0213 (2)
C4	0.76971 (17)	0.16687 (12)	0.60074 (6)	0.0223 (2)
H4	0.9026	0.0993	0.5703	0.027*
C5	0.96435 (17)	0.12171 (13)	0.73471 (6)	0.0240 (2)
H5	1.1005	0.0524	0.7070	0.029*

C4A	0.77384 (17)	0.19200 (12)	0.68915 (6)	0.0217 (2)
C6	0.95376 (17)	0.15324 (13)	0.81971 (6)	0.0256 (2)
H6	1.0835	0.1068	0.8504	0.031*
C7	0.75272 (18)	0.25331 (13)	0.86075 (6)	0.0264 (2)
H7	0.7472	0.2744	0.9193	0.032*
C8	0.56165 (18)	0.32215 (13)	0.81749 (6)	0.0251 (2)
H8	0.4243	0.3888	0.8458	0.030*
C8A	0.57482 (17)	0.29175 (12)	0.73184 (6)	0.0219 (2)
C31	0.59517 (17)	0.20132 (12)	0.46715 (6)	0.0232 (2)
C34	0.22002 (17)	0.29462 (12)	0.30817 (6)	0.0216 (2)
H34	0.0821	0.3485	0.3413	0.026*
C341	0.21746 (16)	0.27545 (12)	0.21730 (6)	0.0215 (2)
C342	0.41939 (17)	0.19665 (13)	0.16727 (6)	0.0238 (2)
H342	0.5605	0.1523	0.1923	0.029*
C343	0.41260 (17)	0.18368 (13)	0.08144 (6)	0.0274 (2)
H343	0.5495	0.1299	0.0478	0.033*
C344	0.20758 (19)	0.24849 (14)	0.04380 (6)	0.0289 (2)
H344	0.2048	0.2399	−0.0153	0.035*
C345	0.00689 (18)	0.32579 (14)	0.09316 (6)	0.0280 (2)
H345	−0.1337	0.3703	0.0678	0.034*
C346	0.01167 (17)	0.33801 (13)	0.17960 (6)	0.0249 (2)
H346	−0.1267	0.3895	0.2132	0.030*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0226 (4)	0.0284 (4)	0.0176 (4)	0.0025 (3)	−0.0017 (3)	−0.0030 (3)
O2	0.0214 (4)	0.0315 (4)	0.0223 (4)	0.0050 (3)	−0.0029 (3)	−0.0030 (3)
O31	0.0276 (4)	0.0432 (4)	0.0196 (4)	0.0139 (3)	−0.0021 (3)	−0.0048 (3)
N32	0.0215 (4)	0.0275 (4)	0.0155 (4)	0.0034 (3)	−0.0008 (3)	−0.0034 (3)
N33	0.0251 (4)	0.0257 (4)	0.0165 (4)	0.0002 (3)	−0.0014 (3)	−0.0022 (3)
C2	0.0229 (5)	0.0227 (5)	0.0181 (5)	−0.0016 (4)	−0.0014 (4)	−0.0013 (3)
C3	0.0215 (5)	0.0223 (5)	0.0192 (5)	−0.0002 (4)	−0.0009 (4)	−0.0011 (4)
C4	0.0226 (5)	0.0231 (5)	0.0201 (5)	−0.0001 (4)	0.0005 (4)	−0.0017 (4)
C5	0.0245 (5)	0.0251 (5)	0.0224 (5)	−0.0026 (4)	−0.0024 (4)	−0.0004 (4)
C4A	0.0236 (5)	0.0218 (5)	0.0199 (5)	−0.0032 (4)	−0.0023 (4)	−0.0002 (3)
C6	0.0279 (5)	0.0270 (5)	0.0232 (5)	−0.0045 (4)	−0.0076 (4)	0.0016 (4)
C7	0.0348 (5)	0.0279 (5)	0.0175 (5)	−0.0066 (4)	−0.0037 (4)	−0.0015 (4)
C8	0.0285 (5)	0.0260 (5)	0.0200 (5)	−0.0021 (4)	0.0004 (4)	−0.0029 (4)
C8A	0.0238 (5)	0.0221 (5)	0.0201 (5)	−0.0031 (4)	−0.0031 (4)	−0.0001 (4)
C31	0.0237 (5)	0.0242 (5)	0.0200 (5)	0.0021 (4)	−0.0006 (4)	−0.0009 (4)
C34	0.0204 (5)	0.0227 (5)	0.0208 (5)	0.0009 (3)	−0.0008 (4)	−0.0013 (3)
C341	0.0233 (5)	0.0212 (5)	0.0200 (5)	−0.0025 (4)	−0.0024 (4)	−0.0008 (4)
C342	0.0218 (5)	0.0270 (5)	0.0222 (5)	−0.0007 (4)	−0.0033 (4)	−0.0009 (4)
C343	0.0272 (5)	0.0315 (5)	0.0225 (5)	−0.0025 (4)	0.0022 (4)	−0.0036 (4)
C344	0.0360 (6)	0.0336 (5)	0.0178 (5)	−0.0057 (4)	−0.0040 (4)	−0.0014 (4)
C345	0.0288 (5)	0.0310 (5)	0.0247 (5)	−0.0011 (4)	−0.0089 (4)	0.0005 (4)
C346	0.0236 (5)	0.0262 (5)	0.0239 (5)	0.0013 (4)	−0.0028 (4)	−0.0015 (4)

Geometric parameters (Å, º)

O1—C8A	1.3749 (11)	C6—H6	0.9500
O1—C2	1.3765 (11)	C7—C8	1.3820 (14)
O2—C2	1.2103 (11)	C7—H7	0.9500
O31—C31	1.2237 (12)	C8—C8A	1.3867 (13)
N32—C31	1.3530 (13)	C8—H8	0.9500
N32—N33	1.3768 (11)	C34—C341	1.4649 (13)
N32—H1	0.857 (15)	C34—H34	0.9500
N33—C34	1.2753 (13)	C341—C346	1.3912 (13)
C2—C3	1.4629 (13)	C341—C342	1.4030 (13)
C3—C4	1.3492 (13)	C342—C343	1.3826 (13)
C3—C31	1.5003 (13)	C342—H342	0.9500
C4—C4A	1.4334 (13)	C343—C344	1.3908 (14)
C4—H4	0.9500	C343—H343	0.9500
C5—C6	1.3790 (13)	C344—C345	1.3890 (15)
C5—C4A	1.4036 (13)	C344—H344	0.9500
C5—H5	0.9500	C345—C346	1.3903 (13)
C4A—C8A	1.3978 (14)	C345—H345	0.9500
C6—C7	1.3960 (14)	C346—H346	0.9500
C8A—O1—C2	123.10 (7)	C8A—C8—H8	120.7
C31—N32—N33	118.22 (8)	O1—C8A—C8	117.65 (8)
C31—N32—H1	121.3 (9)	O1—C8A—C4A	120.69 (8)
N33—N32—H1	120.5 (9)	C8—C8A—C4A	121.66 (9)
C34—N33—N32	116.05 (8)	O31—C31—N32	123.05 (9)
O2—C2—O1	116.32 (8)	O31—C31—C3	120.11 (9)
O2—C2—C3	126.92 (8)	N32—C31—C3	116.83 (8)
O1—C2—C3	116.76 (8)	N33—C34—C341	119.21 (8)
C4—C3—C2	120.21 (9)	N33—C34—H34	120.4
C4—C3—C31	117.51 (8)	C341—C34—H34	120.4
C2—C3—C31	122.28 (8)	C346—C341—C342	119.23 (9)
C3—C4—C4A	121.77 (9)	C346—C341—C34	119.47 (8)
C3—C4—H4	119.1	C342—C341—C34	121.30 (9)
C4A—C4—H4	119.1	C343—C342—C341	119.88 (9)
C6—C5—C4A	119.97 (9)	C343—C342—H342	120.1
C6—C5—H5	120.0	C341—C342—H342	120.1
C4A—C5—H5	120.0	C342—C343—C344	120.75 (9)
C5—C4A—C8A	118.69 (9)	C342—C343—H343	119.6
C5—C4A—C4	123.84 (9)	C344—C343—H343	119.6
C8A—C4A—C4	117.47 (9)	C345—C344—C343	119.56 (9)
C5—C6—C7	120.12 (9)	C345—C344—H344	120.2
C5—C6—H6	119.9	C343—C344—H344	120.2
C7—C6—H6	119.9	C344—C345—C346	120.04 (9)
C8—C7—C6	121.01 (9)	C344—C345—H345	120.0
C8—C7—H7	119.5	C346—C345—H345	120.0
C6—C7—H7	119.5	C341—C346—C345	120.54 (9)
C7—C8—C8A	118.53 (9)	C341—C346—H346	119.7

C7—C8—H8	120.7	C345—C346—H346	119.7
C31—N32—N33—C34	177.57 (7)	C4—C4A—C8A—O1	−0.84 (14)
C8A—O1—C2—O2	179.69 (7)	C5—C4A—C8A—C8	−0.11 (14)
C8A—O1—C2—C3	−0.40 (13)	C4—C4A—C8A—C8	179.54 (8)
O2—C2—C3—C4	179.63 (9)	N33—N32—C31—O31	−1.83 (15)
O1—C2—C3—C4	−0.27 (13)	N33—N32—C31—C3	178.66 (7)
O2—C2—C3—C31	−0.41 (16)	C4—C3—C31—O31	−2.44 (14)
O1—C2—C3—C31	179.69 (7)	C2—C3—C31—O31	177.61 (9)
C2—C3—C4—C4A	0.36 (15)	C4—C3—C31—N32	177.08 (7)
C31—C3—C4—C4A	−179.59 (7)	C2—C3—C31—N32	−2.87 (14)
C6—C5—C4A—C8A	−0.67 (14)	N32—N33—C34—C341	178.28 (7)
C6—C5—C4A—C4	179.70 (8)	N33—C34—C341—C346	−179.53 (8)
C3—C4—C4A—C5	179.82 (8)	N33—C34—C341—C342	−0.13 (14)
C3—C4—C4A—C8A	0.18 (15)	C346—C341—C342—C343	0.63 (14)
C4A—C5—C6—C7	0.70 (14)	C34—C341—C342—C343	−178.78 (8)
C5—C6—C7—C8	0.06 (14)	C341—C342—C343—C344	0.20 (15)
C6—C7—C8—C8A	−0.82 (14)	C342—C343—C344—C345	−0.51 (15)
C2—O1—C8A—C8	−179.39 (7)	C343—C344—C345—C346	−0.01 (15)
C2—O1—C8A—C4A	0.97 (14)	C342—C341—C346—C345	−1.15 (14)
C7—C8—C8A—O1	−178.79 (7)	C34—C341—C346—C345	178.27 (8)
C7—C8—C8A—C4A	0.85 (15)	C344—C345—C346—C341	0.85 (15)
C5—C4A—C8A—O1	179.51 (8)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N32—H1···O2	0.857 (15)	2.062 (15)	2.7238 (10)	133.5 (12)
C34—H34···O2^{i}	0.95	2.54	3.4417 (11)	159
C4—H4···O31	0.95	2.40	2.7415 (11)	101
C4—H4···O31^{ii}	0.95	2.28	3.1377 (12)	149
C5—H5···O31^{ii}	0.95	2.57	3.3456 (12)	139
C346—H346···O1^{i}	0.95	2.63	3.5195 (11)	156

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