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

In the paper by Gomes et al. [Acta Cryst. (2019), E75, 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. E75, 1403–1410.
Crystal structures and Hirshfeld surface analyses of \((E)-N'\text{-}\text{benzylidene}-2\text{-oxo-}2\text{H}-\text{chromene-3-carbohydrazide}\) and the disordered hemi-DMSO solvate of \((E)-2\text{-oxo-}N'\text{-}(3,4,5\text{-trimethoxybenzylidene})-2\text{H}-\text{chromene-3-carbohydrazide}:\) lattice energy and intermolecular interaction energy calculations for the former.

**Corrigendum**

Ligia R. Gomes, John Nicolson Low, James L. Wardell, Camila Capelini, José Daniel Figueroa Villar, Vitória R.F. Câmara, Edson F. da Silva and Samir A. Carvalho

\(\text{(E)-2-Oxo-}N'\text{-}(3,4,5\text{-trimethoxybenzylidene})-2\text{H}-\text{chromene-3-carbohydrazide dimethyl sulfoxide hemisolvate (I)}\)

**Crystal data**

\[
\begin{align*}
C_{20}H_{18}N_2O_6\cdot0.5C_{2}H_{6}OS & \quad F(000) = 1768 \\
M_r &= 421.43 \\
Monoclinic, \text{ C2/c} & \\
a = 33.0258 (7) \text{ Å} & \\
b = 5.4412 (1) \text{ Å} & \\
c = 22.4342 (4) \text{ Å} & \\
\beta &= 107.203 (2) ^\circ \\
V &= 3851.07 (13) \text{ Å}^3 \\
Z &= 8
\end{align*}
\]

**Data collection**

- Rigaku FRE+ equipped with VHF Varimax confocal mirrors and an AFC12 goniometer and HyPix 6000 detector
diffraclmeter
- Radiation source: Rotating Anode, Rigaku FRE+
- Confocal mirrors, VHF Varimax monochromator
- Detector resolution: 10 pixels mm\(^{-1}\)
- profile data from \(\omega\)-scans

**Absorption correction:**

- Gaussian (CrysAlisPro; Rigaku OD, 2019)
- \(T_{\text{min}} = 0.837, \ T_{\text{max}} = 1.000\)
- 22915 measured reflections
- 4381 independent reflections
- 3983 reflections with \(I > 2\sigma(I)\)

**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

---

*Acta Cryst. (2019). E75, 1952* [https://doi.org/10.1107/S2056989019014890]
\[ w = \frac{1}{[\sigma(F_o^2) + (0.0456P)^2] + 2.9167P} \]
\[ \text{where } P = (F_o^2 + 2F_c^2)/3 \]
\[ \Delta \rho_{\text{max}} = 0.31 \text{ e Å}^{-3} \]
\[ \Delta \rho_{\text{min}} = -0.30 \text{ e Å}^{-3} \]
\[(\Delta \sigma)_{\text{max}} = 0.001\]

**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) |
| O3     | 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) | 0.04001 (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*      |
### 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) | 0.0040 (3) | 0.0002 (3) | −0.0066 (3) |
| O31| 0.0143 (3) | 0.0207 (4) | 0.0198 (4) | 0.0036 (3) | 0.0015 (3) | −0.0017 (3) |
| O343| 0.0150 (3) | 0.0195 (4) | 0.0151 (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) | 0.0225 (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) | 0.0077 (4) | 0.0025 (3) | 0.0006 (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) | 0.000664 (18) | 0.00770 (19) | -0.000993 (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, °)**

| Bond/Angle/Dihedral | Distance/Angle | Distance/Angle | Distance/Angle | Distance/Angle | Distance/Angle | Distance/Angle |
|---------------------|----------------|----------------|----------------|----------------|----------------|----------------|
| O1—C2               | 1.3702 (12)    | C34—C341       | 1.4629 (14)    |                 |                |                |
| O1—C8A              | 1.3747 (12)    | C34—H34        | 1.3953 (14)    |                 |                |                |
| O2—C2               | 1.2133 (12)    | C341—C342      | 1.3955 (14)    |                 |                |                |
| O31—C31             | 1.2234 (13)    | C341—C346      | 1.3894 (13)    |                 |                |                |
| O343—C343           | 1.3631 (12)    | C342—C343      | 0.9500         |                 |                |                |
| O343—C431           | 1.4280 (12)    | C342—H342      | 1.4028 (14)    |                 |                |                |
| O344—C441           | 1.4356 (12)    | C344—C345      | 1.3921 (14)    |                 |                |                |
| O345—C345           | 1.3635 (12)    | C345—H346      | 0.9500         |                 |                |                |
| N32—C31             | 1.3543 (13)    | C346—C346      | 0.9800         |                 |                |                |
| N32—N33             | 1.3793 (11)    | C346—H346      | 1.483 (16)     |                 |                |                |
| N32—H32             | 0.870 (16)     | C431—H43A      | 1.3955 (14)    |                 |                |                |
| N33—C34             | 1.2753 (14)    | C431—H43B      | 0.9800         |                 |                |                |
| C2—C3               | 1.4647 (13)    | C431—H43C      | 0.9800         |                 |                |                |
| C3—C4               | 1.3547 (14)    | C441—H41A      | 0.9800         |                 |                |                |
| C3—C31              | 1.5056 (13)    | C441—H41B      | 0.9800         |                 |                |                |
| C4—C4A              | 1.4340 (13)    | C441—H41C      | 0.9800         |                 |                |                |
| C4—H4               | 0.9500         | C451—H51A      | 0.9800         |                 |                |                |
| C5—C6               | 1.3840 (15)    | C451—H51B      | 0.9800         |                 |                |                |
| C5—C4A              | 1.4057 (14)    | C451—H51C      | 0.9800         |                 |                |                |
| C5—H5               | 0.9500         | S1S—O1S        | 1.483 (16)     |                 |                |                |
| C4A—C8A             | 1.3935 (14)    | S1S—C2S        | 1.775 (7)      |                 |                |                |
| C6—C7               | 1.3965 (16)    | C1S—H1SA       | 0.9800         |                 |                |                |
| C6—H6               | 0.9500         | C1S—H1SB       | 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         |                 |                |                |
| C2—O1               | 122.80 (8)     | C341—H342      | 120.5          |                 |                |                |
| C343—O343—C431      | 116.52 (8)     | O343—C343      | 124.14 (9)     |                 |                |                |
| C344—O344—C441      | 113.00 (8)     | O343—C344      | 115.17 (8)     |                 |                |                |
| C345—O345—C451      | 116.90 (8)     | C342—C343      | 120.69 (9)     |                 |                |                |
| C31—N32—N33         | 120.41 (9)     | O344—C344      | 120.16 (9)     |                 |                |                |
| C31—N32—H32         | 117.6 (10)     | O344—C345      | 120.05 (9)     |                 |                |                |
| N33—N32—H32         | 121.7 (10)     | C345—C344      | 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—H346 120.0
C4—C3—C2 119.74 (9)  C345—C346—C341 119.92 (10)
C4—C3—C31 117.95 (9)  O343—C431—H43A 109.5
C2—C3—C31 122.31 (9)  O343—C431—H43B 109.5
C3—C4—C4A 121.44 (9)  O343—C431—H43C 109.5
C3—C4—H4 119.3  H43A—C431—H43B 109.5
C4A—C4—H4 119.3  O344—C441—H41A 109.5
C6—C5—C4A 119.72 (10)  O344—C441—H41B 109.5
C6—C5—H5 120.1  O344—C441—H41C 109.5
C4A—C5—H5 120.1  S1S—C1S—H1SA 109.5
C8A—C4A—C5 118.30 (9)  S1S—C1S—C2S 105.5 (10)
C8A—C4A—C4 117.88 (9)  S1S—C1S—C1S 109.8 (19)
C5—C4A—C4 123.81 (9)  S1S—C2S—H2SA 109.5
C5—C6—C7 120.56 (10)  S1S—C2S—H2SB 109.5
C5—C6—H6 119.7  S1S—C2S—H2SC 109.5
C7—C6—H6 119.7  N32—N33—C34—C341 177.68 (10)
C8—C7—C6 120.80 (9)  N33—C34—C341—C342 9.81 (18)
C8—C7—H7 119.6  N33—C34—C341—C346 −169.23 (11)
C6—C7—H7 119.6  C346—C341—C342—C343 −1.33 (16)
C7—C8—C8A 117.99 (10)  C34—C341—C342—C343 179.66 (10)
C7—C8—H8 121.0  H51B—C451—H51C 109.5
C8A—C8—H8 121.0  H51B—C451—H51A 109.5
O1—C8A—C8 116.63 (9)  H51B—C451—H51A 109.5
O1—C8A—C4A 120.73 (9)  C346—C341—C342—C343 179.66 (10)
C8—C8A—C4A 122.62 (9)  C34—C341—C342—C343 179.66 (10)
O31—C31—N32 124.05 (9)  C34—C341—C342—C343 179.66 (10)
O31—C31—C3 121.09 (9)  C34—C341—C342—C343 179.66 (10)
N32—C31—C3 114.86 (9)  C34—C341—C342—C343 179.66 (10)
N33—C34—C341 121.94 (10)  C34—C341—C342—C343 179.66 (10)
N33—C34—H34 119.0  C34—C341—C342—C343 179.66 (10)
C341—C34—H34 119.0  C34—C341—C342—C343 179.66 (10)
C342—C341—C346 120.85 (9)  C342—C341—C342—C343 179.66 (10)
C342—C341—C34 121.44 (9)  C342—C341—C342—C343 179.66 (10)
C346—C341—C34 117.71 (9)  C342—C341—C342—C343 179.66 (10)
C343—C342—C341 118.94 (9)  C342—C341—C342—C343 179.66 (10)
C343—C342—H342 120.5  C342—C341—C342—C343 179.66 (10)

| 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—C345 5.20 (13)
C5—C6—C7—C8 −1.25 (15) O343—C343—C344—C344 177.09 (9)
C6—C7—C8—C8A −0.72 (15) O343—C343—C344—C343 174.41 (9)
C2—O1—C8A—C8 178.49 (9) C342—C343—C344—O344 −174.41 (9)
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—C345 176.88 (9)
C4—C4A—C8A—O1 0.08 (14) O344—C344—C345—C346 −3.31 (15)
C5—C4A—C8A—C8 0.52 (15) O344—C344—C345—C346 −179.17 (10)
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, °)

| D—H···A         | D—H  | H···A  | D···A  | D—H···A |
|----------------|-------|--------|--------|---------|
| N32—H32···O2   | 0.870 | 1.955  | 2.6878 | 141.0   |
| C441—H41C···O345i | 0.98  | 2.58   | 3.4772 | 152     |
| C451—H51A···O1u  | 0.98  | 2.65   | 3.4463 | 138     |
| C34—H34···O1S   | 0.95  | 2.57   | 3.30   | 134     |
| C34—H34···O1Si  | 0.95  | 2.63   | 3.34   | 133     |
| C34—H34···S1S   | 0.95  | 2.69   | 3.6158 | 166     |
| C431—H43C···O343iii | 0.98  | 2.50   | 3.2505 | 133     |
| C2S—H2S···N32v  | 0.98  | 2.61   | 3.3000 | 127     |
| C4—H4···O31     | 0.95  | 2.45   | 2.7761 | 100     |
| C4—H4···O31v    | 0.95  | 2.38   | 3.2415 | 150     |
| C5—H5···O31v    | 0.95  | 2.59   | 3.3931 | 143     |
| C431—H43B···Cg3vi | 0.98  | 2.73   | 3.5882 | 147     |
| C451—H51B···Cg3vi | 0.98  | 2.95   | 3.8562 | 155     |
| C451—H51C···Cg2iii | 0.98  | 2.83   | 3.6883 | 147     |
| C31—O31···Cg1ii | 0.0   | 0      | 3.3971 | 90      |

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+1/2; (v) −x+1, −y, −z+1; (vi) x, y−1, z; (vii) −x+1, −y+1, −z+1.

(E)-N'-Benzyldiene-2-oxo-2H-chromene-3-carbohydrazide (II)

Crystal data

| C17H12N2O3 | Triclinic, P1̅ |
|-------------|----------------|
| Mr = 292.29 | a = 5.6715 (1) Å |

Acta Cryst. (2019). E75, 1952
sup-7

$\beta = 7.4164 (1) \text{ Å}$
$\gamma = 82.961 (2)^{\circ}$
$V = 663.60 (2) \text{ Å}^3$

Cell parameters from 8290 reflections

$\theta = 6.0–70.3^{\circ}$
$\mu = 0.84 \text{ mm}^{-1}$
$T = 100 \text{ K}$

Plate, colourless

$0.22 \times 0.12 \times 0.05 \text{ mm}$

Data collection

Rigaku 007HF equipped with Varimax confocal
mirrors and an AFC11 goniometer and HyPix
6000 detector
diffractometer

Absorption correction: multi-scan
(CrysAlisPro; Rigaku OD, 2019)

$T_{\text{min}} = 0.930$, $T_{\text{max}} = 1.000$

11641 measured reflections

2352 independent reflections

2250 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.027$

$\theta_{\text{max}} = 67.1^{\circ}$, $\theta_{\text{min}} = 5.6^{\circ}$

$h = -6^{\rightarrow}6$

$k = -8^{\rightarrow}8$

$l = -19^{\rightarrow}19$

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

$w = 1/[\sigma^2(F^2_c) + (0.0858P)^2 + 0.127P]$

where $P = (F^2_c + 2F^2)3$

$\Delta \rho_{\text{max}} = 0.23 \text{ e Å}^{-3}$

$\Delta \rho_{\text{min}} = -0.19 \text{ e Å}^{-3}$

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 ($\text{Å}^2$)

|   | $x$       | $y$       | $z$       | $U_{\text{iso}}/U_{\text{eq}}$ |
|---|-----------|-----------|-----------|-------------------------------|
| 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*       |

Acta Cryst. (2019). E75, 1952
| 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, °)

| Bond/Angle                           | Distance/ Å | Angle/ °   |
|--------------------------------------|-------------|------------|
| 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) | C34—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 |

| Bond/Angle                           | Distance/ Å | Angle/ °   |
|--------------------------------------|-------------|------------|
| C8A—O1—C2                           | 123.10 (7)  | C8A—C8—H8 120.7 |
| C8A—O1—C2                           | 118.22 (8)  | O1—C8A—C8 117.65 (8) |
| C31—N32—N33                         | 118.22 (8)  | O1—C8A—C4A 120.69 (8) |
| C31—N32—H1                          | 121.3 (9)   | O1—C8A—C4A 121.66 (9) |
| C31—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—C1                            | 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       | C343—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 |

*Acta Cryst. (2019). E75, 1952*
Hydrogen-bond geometry (Å, °)

|   | 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···O2i | 0.95 | 2.54 | 3.4417 (11) | 159 |
| C4—H4···O3i | 0.95 | 2.40 | 2.7415 (11) | 101 |
| C4—H4···O3i | 0.95 | 2.28 | 3.1377 (12) | 149 |
| C5—H5···O3i | 0.95 | 2.57 | 3.3456 (12) | 139 |
| C346—H346···O1i | 0.95 | 2.63 | 3.5195 (11) | 156 |

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