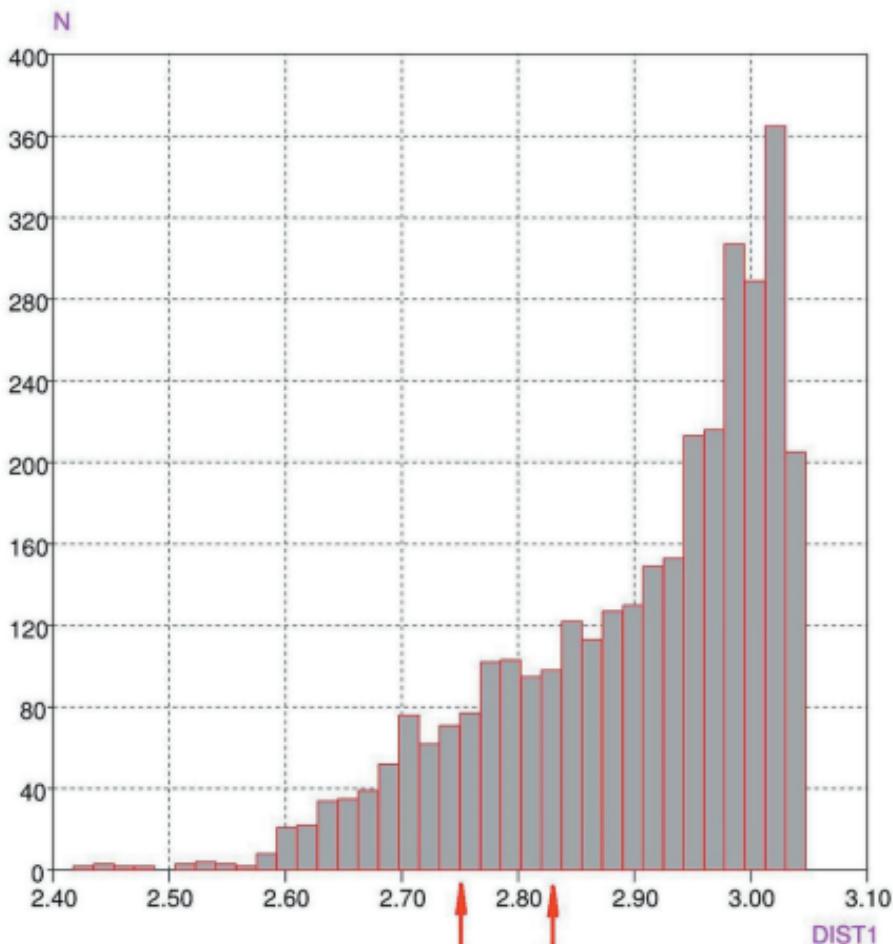


## **Structural aspects of two alpha-dihydrazone displaying a complete survey of intermolecular interactions**

### Supplementary Fig. S1

Distribution of short O...O contacts reported in the CSD and organized by VISTA in the CSD package. Red arrows indicate the values found in (I).

DIST1



**Plot Data**  
File=cq\_temp0  
Test=1  
Tot.Obs.=3315  
Obs.=3305  
Supp.=10

**X-axis**  
Min.=2.429  
Max.=3.040  
Range=0.611  
Mean=2.901  
Mean SE=0.002  
Sample SD=0.117

**Histogram**  
Median=2.936  
Skew=-0.904  
Quantile=10.000  
LQ=2.722  
HQ=3.025  
Bin Width=0.018  
Max. Bin =365.000

## **Supplementary Material for Submission fp3020**

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### **IR and NMR data:**

#### **(I):**

UV-visible spectrum in THF  $1.16 \times 10^{-5}$  mol/L,  $\lambda_{\text{máx},\text{nm}}(\log \varepsilon)$ :  $\lambda_1$ : 434(4.49),  $\lambda_2$ : 394(4.00),  $\lambda_3$ : 297(3.95),  $\lambda_4$ : 245(4.23). IR spectrum on KBr pellet: v(N-H): 3285s v(C-H) Ar.: 3105w, 3056w; v(C-H) Aliph.: 2976w; v(C=O): 1730s; v(C=N) or v(C=C); 1610s, 1578s, 1497s.  $^1\text{H}$  NMR (400 MHz, DMSO-d<sub>6</sub>)  $\delta$ (ppm): 10.97 (s, 1H, N-H), 10.78 (s, 1H, N-H), 8.25 – 8.07 (m, 3H, CH, Ar.), 7.69 (d,  $J$  = 13.8 Hz, 2H, CH Ar.), 7.43 (d,  $J$  = 8.6 Hz, 2H, CH Ar.), 7.00 (s, 1H, CH Ar.), 4.48 (q,  $J$  = 6.8 Hz, 2H,  $\text{CH}_2\text{CH}_3$ ), 3.60 (s, 2H, -CH<sub>2</sub>-CH<sub>2</sub>O THF), 2.32 (s, 3H, CH<sub>3</sub>-), 1.76 (s, 2H, CH<sub>2</sub>CH<sub>2</sub>, THF), 1.36 (t,  $J$  = 6.3 Hz, 3H CH<sub>3</sub>CH<sub>2</sub>O-).  $^{13}\text{C}$  NMR (101 MHz, DMSO-d<sub>6</sub>)  $\delta$ (ppm) 163.68, 150.09, 146.65, 140.98, 140.77, 140.65, 140.40, 136.93, 132.14, 126.09, 119.84, 115.64, 113.41, 67.38(THF), 62.12, 25.48(THF), 14.39, 10.52.

#### **(II)**

IR spectrum on KBr pellet: v(N-H): 3308m, 3295m: v(C-H) Ar.: 3111w, v(C-H) Aliph.: 2924w; v(C=N) or v(C=C); 1612s, 1575s.  $^1\text{H}$  NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  14.78 (s, 1H, N-H), 12.76 (s, 1H, N-H), 7.05 -7.44 (m, 9H, C-H Ar. and C-H methine), 2.48 (s, 3H, CH<sub>3</sub>).  $^{13}\text{C}$  NMR not presented, because of its poor quality due to low solubility of (II) in CDCl<sub>3</sub>

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