

Experimental and computational evidence for stabilising parallel, off-set $\pi[C(=O)N(H)N=C]\cdots\pi(\text{phenyl})$ interactions in acetohydrazide derivatives†

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ESI Table 2. Compilation of literature structures featuring $\pi[C(=O)N(H)N=C]\cdots\pi(\text{phenyl})$ interactions in acetohydrazide derivatives – *anti*-amides

Compound Spectrum SmartFormula Report

Analysis Info

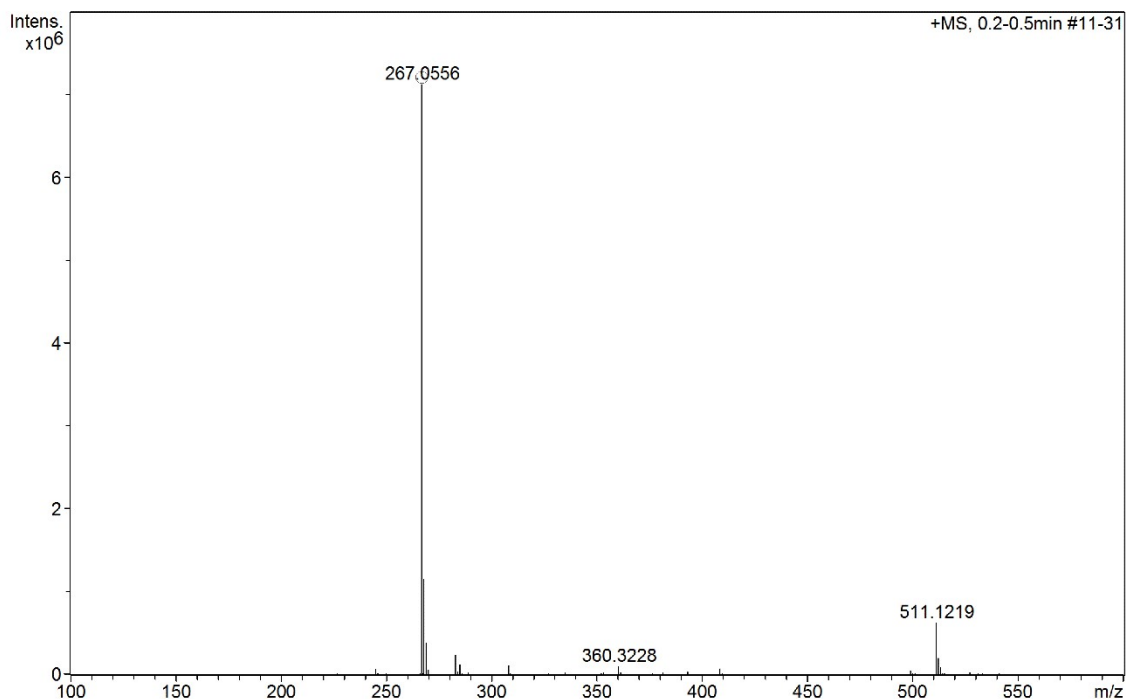
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Comment

Acquisition Date 12/1/2021 10:15:14 AM
Operator Vinicius
Instrument compact 8255754.10035

Acquisition Parameter

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Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

+MS, 0.2-0.5min #11-31



Meas. m/z # Ion Formula	m/z err [ppm]	Mean err rdb [ppm]	N-Rule	e ⁻ Conf	mSigma	Std I	Std	Mean m/z	Std I	VarNorm	Std m/z	Diff	Std Comb Dev
267.055634 1 C ₁₃ H ₁₂ N ₂ NaOS	267.056255	2.3	2.4	8.5	ok	even	3.1	5.0	n.a.	n.a.	n.a.	n.a.	n.a.

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by: Vinicius

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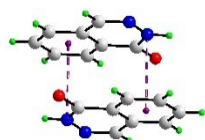
ESI Figure 1. The HRMS spectrum measured for N'-[(1*E*)-phenylmethylidene]-2-(thiophen-2-yl)acetohydrazide (**1**).

ESI Table 1. Compilation of literature structures featuring $\pi[\text{C}(\text{=O})\text{N}(\text{H})\text{N}=\text{C}] \cdots \pi(\text{phenyl})$ interactions in acetohydrazide derivatives – *syn*-amides. Within each supramolecular aggregation pattern, aggregates are ordered in terms of REFCODE.

Centrosymmetric dimer:

s1. GIRPON phthalazin-1(2H)-one picric acid (1/1)

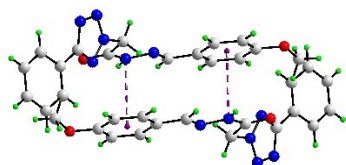
H. S. Yathirajan, B. Narayana, M. T. Swamy, B. K. Sarojini and M. Bolte, *Acta Crystallogr., Sect. E: Cryst. Commun.*, 2008, **64**, o119, <https://doi.org/10.1107/S1600536807063362>



$d(\text{HN} \cdots \text{Cg}) = 3.36 \text{ \AA}$; $\text{C} \cdots \text{C} = 3.30 \text{ \AA}$; $\text{N} \cdots \text{C} = 3.39 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 2.2^\circ$;
sum of angles about N(H) = 359.9°

s2. WODXIZ N'-[(4-methoxyphenyl)methylidene]-2-(5-phenyl-2H-tetrazol-2-yl)acetohydrazide

M. M. Naseer, M. Hussain, A. Bauzá, K. M. Lo and A. Frontera, *ChemPlusChem*, 2018, **83**, 881-885, <https://doi.org/10.1002/cplu.201800329>

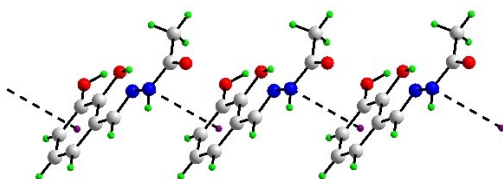


$d(\text{HN} \cdots \text{Cg}) = 3.40 \text{ \AA}$; $\text{C} \cdots \text{C} = 3.35 \text{ \AA}$; $\text{N} \cdots \text{C} = 3.49 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 3.6^\circ$;
sum of angles about N(H) = 360.0°

Linear chain:

s3. BOWQIP N'-(2,3-dihydroxybenzylidene)acetohydrazide

D. Sadhukhan, M. Maiti, G. Pilet, A. Bauzá, A. Frontera and S. Mitra, *Eur. J. Inorg. Chem.*, 2015, 1958-1972, <https://doi.org/10.1002/ejic.201500030>

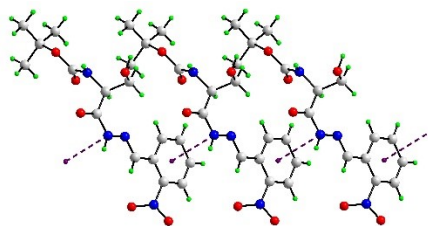


$d(\text{HN} \cdots \text{Cg}) = 3.33 \text{ \AA}$; $\text{C} \cdots \text{C} = 3.40 \text{ \AA}$; $\text{N} \cdots \text{C} = 3.34 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 7.1^\circ$;
sum of angles about N(H) = 359.4°

s4. IPUWOG t-butyl (3-hydroxy-1-(2-(2-nitrobenzylidene)hydrazino)-1-oxopropan-2-yl)carbamate

R. A. Howie, M. V. N. de Souza, A. Pinheiro, C. R. Kaiser, J. L. Wardell and S. M. S. V. Wardell, *Z.*

Kristallogr. Cryst. Mater., 2011, **226**, 483-491, <https://doi.org/10.1524/zkri.2011.1359>



$d(\text{HN}\cdots\text{Cg}) = 3.45 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.34 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.39 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 3.6^\circ$;

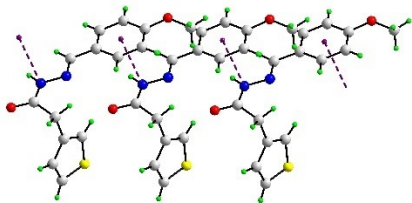
sum of angles about $\text{N}(\text{H}) = 358.2^\circ$

s5. LOHTUA N'-[(4-methoxyphenyl)methylidene]-2-(thiophen-3-yl)acetohydrazide

T. Vu Quoc, L. Nguyen Ngoc, D. Tran Thi Thuy, M. Vu Quoc, T. Vuong Nguyen, Y. Oanh Doan Thi

and L. Van Meervelt, *Acta Crystallogr., Sect. E: Cryst. Commun.*, 2019, **75**, 1090-1095,

<https://doi.org/10.1107/S2056989019008892>



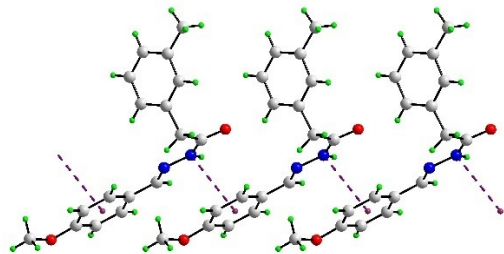
$d(\text{HN}\cdots\text{Cg}) = 3.43 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.50 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.48 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 9.1^\circ$;

sum of angles about $\text{N}(\text{H}) = 360.0^\circ$

s6. PECVEA (E)-N'-(4-methoxybenzylidene)-2-m-tolylacetohydrazide

A. S. Praveen, J. P. Jasinski, A. C. Keeley, H. S. Yathirajan and B. Narayana, *Acta Crystallogr., Sect. E:*

Cryst. Commun., 2012, **68**, o3435, <https://doi.org/10.1107/S1600536812047113>



$d(\text{HN}\cdots\text{Cg}) = 3.43 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.40 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.46 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 4.4^\circ$;

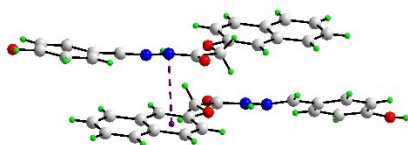
sum of angles about $\text{N}(\text{H}) = 360.0^\circ$

ESI Table 2. Compilation of literature structures featuring $\pi[C(=O)N(H)N=C]\cdots\pi(\text{phenyl})$ interactions in acetohydrazide derivatives – *anti*-amides. Within each supramolecular aggregation pattern, aggregates are ordered in terms of REFCODE.

Non-symmetric two-molecule aggregates:

a1. CEGFAX N'-(4-hydroxybenzylidene)-2-(2-naphthyloxy)acetohydrazide

R. Kant, V. K. Gupta, K. Kapoor, S. Samshuddin, B. Narayana and B. K. Sarojini, *Acta Crystallogr., Sect. E: Cryst. Commun.*, 2012, **68**, o2923-o2924, <https://doi.org/10.1107/S1600536812038408>



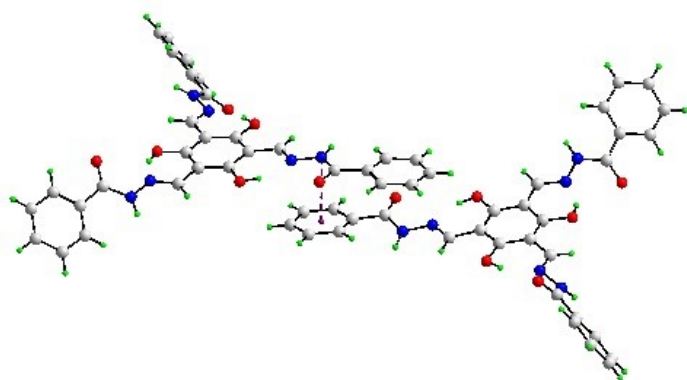
Two independent molecules which associate via a single interaction

$d(\text{HN}\cdots\text{Cg}) = 3.43 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.67 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.59 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 11.8^\circ$;

sum of angles about N(H) = 360.0°

a2. BACBOZ N'-(3,5-bis((benzoylhydrazono)methyl)-2,4,6-trihydroxybenzylidene)benzohydrazide methanol solvate

J. S. Foster, J. M. Żurek, N. M. S. Almeida, W. E. Hendriksen, V. A. A. le Sage, V. Lakshminarayanan, A. L. Thompson, R. Banerjee, R. Eelkema, H. Mulvana, M. J. Paterson, J. H. van Esch and G. O. Lloyd, *J. Am. Chem. Soc.*, 2015, **137**, 14236-14239, <https://doi.org/10.1021/jacs.5b06988>



Non-symmetric dimer formed by two independent molecules

$d(\text{HN}\cdots\text{Cg}) = 3.37 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.28 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.25 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 5.3^\circ$;

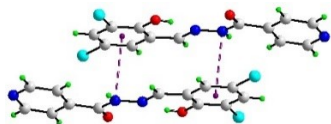
sum of angles about N(H) = 360.0°

Centrosymmetric dimeric aggregates:

a3. AQEMIT N'-(3,5-dichloro-2-hydroxybenzylidene)isonicotinohydrazide

J. Xu, Y.-Q. Shu and P. Hu, *Z. Kristallogr. - New Cryst. Struct.*, 2011, **226**, 63-64,

<https://doi.org/10.1524/ncrs.2011.0031>



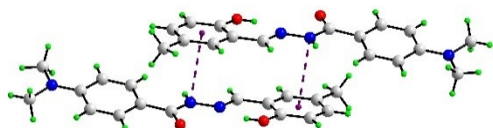
$d(\text{HN}\cdots\text{Cg}) = 3.40 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.34 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.39 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 0.8^\circ$;

sum of angles about N(H) = 360.0°

a4. CABXAH 4-(dimethylamino)-N'-(2-hydroxy-5-methylbenzylidene)benzohydrazide

X.-F. Meng, W.-N. Li and J.-J. Ma, *J. Chil. Chem. Soc.*, 2014, **59**, 2647-2651, [https://doi.org/10.4067/S0717-](https://doi.org/10.4067/S0717-97072014000400004)

[97072014000400004](https://doi.org/10.4067/S0717-97072014000400004)



Two independent molecules: only one forms the interaction

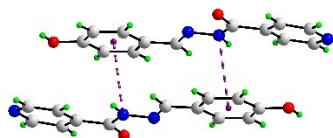
$d(\text{HN}\cdots\text{Cg}) = 3.43 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.54 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.44 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 7.2^\circ$;

sum of angles about N(H) = 360.0°

a5. CASQUJ N'-(4-hydroxybenzylidene)isonicotinohydrazide

Q.-L. Deng, M. Yu, X. Chen, C.-H. Diao, Z.-L. Jing and Z. Fan, *Acta Crystallogr., Sect. E: Cryst.*

Commun., 2005, **61**, o2545-o2546, <https://doi.org/10.1107/S1600536805022191>



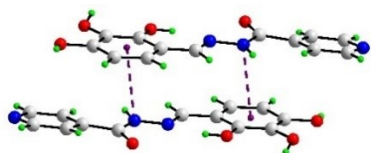
$d(\text{HN}\cdots\text{Cg}) = 3.45 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.47 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.51 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 3.8^\circ$;

sum of angles about N(H) = 359.9°

a6. CEDRUA (E)-N'-(2,3,4-trihydroxybenzylidene)isonicotinohydrazide dihydrate

H. S. Naveenkumar, A. Sadikun, P. Ibrahim, J. H. Goh and H.-K. Fun, *Acta Crystallogr., Sect. E: Cryst.*

Commun., 2010, **66**, o3017-o3018, <https://doi.org/10.1107/S1600536810043965>

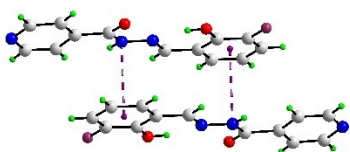


$d(\text{HN}\cdots\text{Cg}) = 3.37 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.41 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.38 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 5.5^\circ$;
sum of angles about $\text{N}(\text{H}) = 359.8^\circ$

a7. FECQEM $\text{N}'\text{-}[(3\text{-fluoro-2-hydroxyphenyl)methylidene}]$ pyridine-4-carbohydrazide

S. Jiajaroen, K. Chainok and F. Kielar, *Acta Crystallogr., Sect. E: Cryst. Commun.*, 2017, **73**, 1151-1153,

<https://doi.org/10.1107/S2056989017009926>

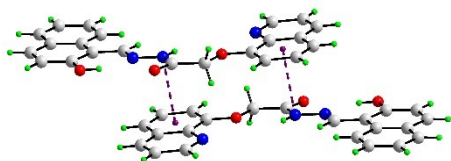


$d(\text{HN}\cdots\text{Cg}) = 3.40 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.35 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.40 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 1.8^\circ$;
sum of angles about $\text{N}(\text{H}) = 360.0^\circ$

a8. FIXQOU (*E*)- $\text{N}'\text{-}[(2\text{-hydroxynaphthalen-1-yl)methylene}]$ -2-(quinolin-8-yloxy)acetohydrazide sesquihydrate

S. Goswami, A. K. Das, K. Aich, A. Manna, H.-K. Fun and C. K. Quah, *Supramol. Chem.*, 2014, **26**, 94-

104, <https://doi.org/10.1080/10610278.2013.826805>



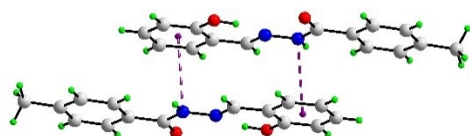
Four independent organic molecules; one associates about a centre of inversion

$d(\text{HN}\cdots\text{Cg}) = 3.31 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.42 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.36 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 6.7^\circ$;
sum of angles about $\text{N}(\text{H}) = 360.0^\circ$

a9. FURCUT $\text{N}'\text{-}[(2\text{-hydroxyphenyl)methylidene}]$ -4-methylbenzohydrazide

S. Ta, M. Ghosh, N. Salam, J. Das, M. Islam, P. Brandão, V. Félix, J. Sanmartin and D. Das, *Appl.*

Organomet. Chem., 2020, **24**, e5823, <https://doi.org/10.1002/aoc.5823>

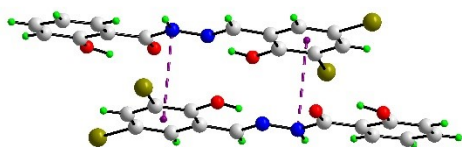


Two independent organic molecules; one associates about a centre of inversion

$d(\text{HN}\cdots\text{Cg}) = 3.29 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.35 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.28 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 2.3^\circ$;
sum of angles about $\text{N}(\text{H}) = 359.9^\circ$

a10. GIGQUJ N-((3,5-dibromo-2-hydroxyphenyl)methylene)-2-hydroxybenzohydrazide methanol solvate

N. Wang, J.-P. Li and Y.-L. Pu, *Chin. J. Struct. Chem.*, 2007, **26**, 547-550.

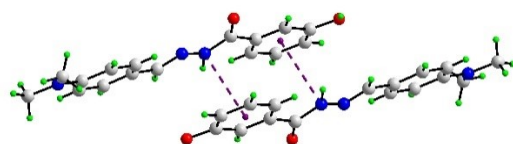


$d(\text{HN}\cdots\text{Cg}) = 3.41 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.43 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.40 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 1.7^\circ$;
sum of angles about $\text{N}(\text{H}) = 359.8^\circ$

a11. GITBER N'-(4-(dimethylamino)benzylidene)-3-hydroxybenzohydrazide

Y. Nie, *Acta Crystallogr., Sect. E: Struct. Cryst. Commun.*, 2008, **64**, o471,

<https://doi.org/10.1107/S160053680800130X>

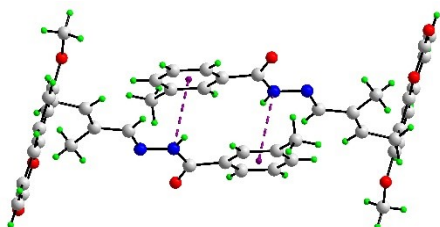


$d(\text{HN}\cdots\text{Cg}) = 3.40 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.71 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.27 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 15.4^\circ$;
sum of angles about $\text{N}(\text{H}) = 358.6^\circ$

a12. GOQLIK N'-((1E,2E)-4-(7-methoxy-2-oxo-2H-chromen-8-yl)-2-methylbut-2-en-1-ylidene)-3-methylbenzohydrazide

X. Yu, Y.-F. Zhao, Y. Qin, J. Yan and Y.-F. Chen, *Z. Kristallogr.-New Cryst. Struct.*, 2019, **234**, 1039-1041,

<https://doi.org/10.1515/ncrs-2019-0249>



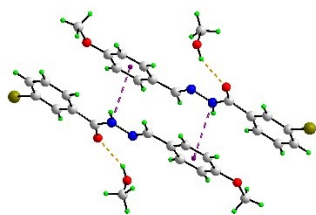
Two independent molecules: one self-associates about a centre of inversion

$d(\text{HN}\cdots\text{Cg}) = 3.45 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.83 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.43 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 20.6^\circ$;
sum of angles about $\text{N}(\text{H}) = 360.0^\circ$

a13. HUCSOO (E)-3-bromo-N'-(4-methoxybenzylidene)benzohydrazide methanol solvate

G.-B. Cao, *Acta Crystallogr., Sect. E: Cryst. Commun.*, 2009, **65**, o2086,

<https://doi.org/10.1107/S1600536809030219>



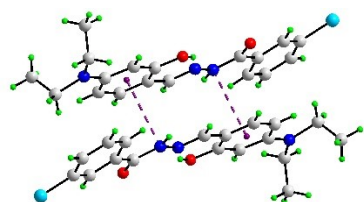
$d(\text{HN}\cdots\text{Cg}) = 3.44 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.61 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.46 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 9.9^\circ$;

sum of angles about N(H) = 359.8°

a14. IJUXIV 3-chloro-N'-(4-(diethylamino)-2-hydroxybenzylidene)benzohydrazide

T.-Y. Li and B.-B. Li, *Acta Crystallogr., Sect. E: Cryst. Commun.*, 2011, **67**, o383,

<https://doi.org/10.1107/S1600536811001218>



Two independent molecules: one self-associates about a centre of inversion

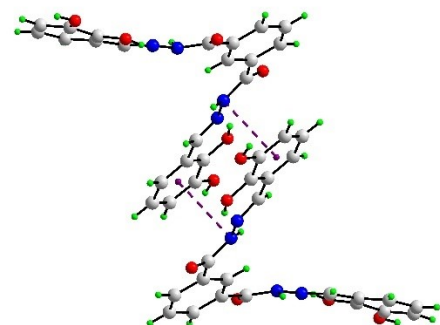
$d(\text{HN}\cdots\text{Cg}) = 3.39 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.58 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.31 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 5.0^\circ$;

sum of angles about N(H) = 360.0°

a15. JOLDOF N'1,N'3-bis(2,3-dihydroxybenzylidene)isophthalohydrazide

S. Sharma, M. S. Hundal, A. Walia, V. Vanita and G. Hundal, *Org. Biomol. Chem.*, 2014, **12**, 4445-4453,

<https://doi.org/10.1039/C4OB00329B>



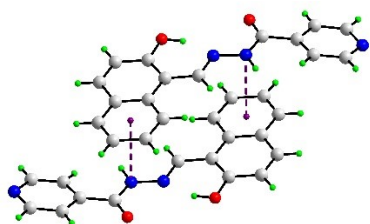
$d(\text{HN}\cdots\text{Cg}) = 3.37 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.46 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.45 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 5.5^\circ$;

sum of angles about N(H) = 359.5°

a16. KAVSEF 2-hydroxyl-1-naphthaldehyde isonicotinoyl hydrazone

D. R. Richardson and P. V. Bernhardt, *J. Biol. Inorg. Chem.*, 1999, **4**, 266-273,

<https://doi.org/10.1007/s007750050312>



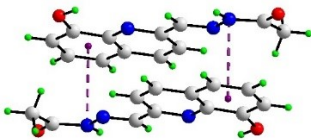
$d(\text{HN}\cdots\text{Cg}) = 3.39 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.29 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.45 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 2.2^\circ$;

sum of angles about N(H) = 359.8°

a17. LOPHAB 2-[(8-hydroxyquinolinyl)methylene]acetohydrazide

L. M. F. Gomes, R. P. Vieira, M. R. Jones, M. C. P. Wang, C. Dyrager, E. M. Souza-Fagundes, J. G. Da Silva, T. Storr and H. Beraldo, *J. Inorg. Biochem.*, 2014, **139**, 106-116,

<https://doi.org/10.1016/j.jinorgbio.2014.04.011>



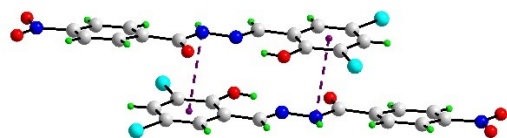
Two independent molecules: one self-associates about a centre of inversion

$d(\text{HN}\cdots\text{Cg}) = 3.29 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.36 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.34 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 5.2^\circ$;

sum of angles about N(H) = 360.0°

a18. LUTWUU N'-(3,5-dichloro-2-hydroxybenzylidene)-4-nitrobenzohydrazide N,N-dimethylformamide solvate

B. Joseph, N. R. Sajitha, M. Sithambaresan, E. B. Seenaa and M. R. P. Kurup, *Acta Crystallogr., Sect. E: Cryst. Commun.*, 2015, **71**, o826-o827, <https://doi.org/10.1107/S2056989015018290>

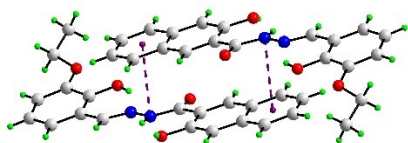


$d(\text{HN}\cdots\text{Cg}) = 3.42 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.43 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.39 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 1.7^\circ$;

sum of angles about N(H) = 359.9°

a19. MIXWUM N'-(3-ethoxy-2-hydroxybenzylidene)-3-hydroxynaphthalene-2-carbohydrazide

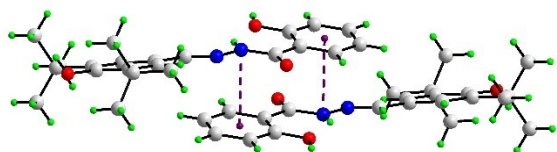
J.-T. Lei, Y.-X. Jiang, L.-Y. Tao, S.-S. Huang and H.-L. Zhang, *Acta Crystallogr., Sect. E: Cryst. Commun.*, 2008, **64**, o909, <https://doi.org/10.1107/S1600536808010933>



$d(\text{HN}\cdots\text{Cg}) = 3.36 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.49 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.36 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 7.8^\circ$;
sum of angles about N(H) = 359.9°

a20. MODQOM N'-(3-ethoxy-2-hydroxybenzylidene)-3-hydroxynaphthalene-2-carbohydrazide methanol solvate

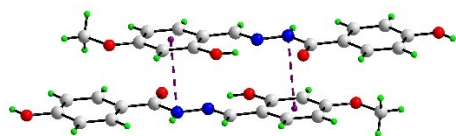
W. A. Yehye, A. Ariffin and S. W. Ng, *Acta Crystallogr., Sect. E: Cryst. Commun.*, 2008, **64**, o1452, <https://doi.org/10.1107/S1600536808020746>



Two independent molecules: only one self-associates about a centre of inversion
 $d(\text{HN}\cdots\text{Cg}) = 3.34 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.39 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.40 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 4.4^\circ$;
sum of angles about N(H) = 360.0°

a21. MOKRUA (E)-4-hydroxy-N'-(2-hydroxy-4-methoxybenzylidene)benzohydrazide monohydrate

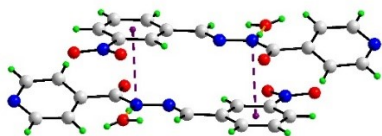
N. Md. Lair, H. Md. Ali and S. W. Ng, *Acta Crystallogr., Sect. E: Cryst. Commun.*, 2009, **65**, o189, <https://doi.org/10.1107/S1600536808042888>



$d(\text{HN}\cdots\text{Cg}) = 3.42 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.37 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.42 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 2.6^\circ$;
sum of angles about N(H) = 360.0°

a22. NEFTEY01 3-nitrobenzaldehyde isonicotinoylhydrazone monohydrate

S. M. S. V. Wardell, J. L. Wardell, J. N. Low, C. Glidewell and M. V. N. de Souza, *Acta Crystallogr., Sect. C: Cryst. Struct. Chem.*, 2007, **63**, o42-o44, <https://doi.org/10.1107/S0108270106050451>

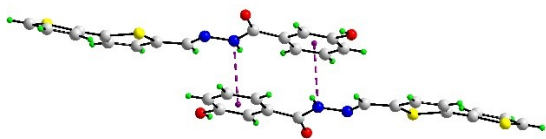


Determination at 120 K

$d(\text{HN}\cdots\text{Cg}) = 3.35 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.33 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.40 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 1.1^\circ$;
sum of angles about $\text{N}(\text{H}) = 360.0^\circ$

a23. NUHSUH $\text{N}'\text{-}((2,2'\text{-bithiophen-5-yl)methylidene})\text{-3-hydroxybenzohydrazide}$

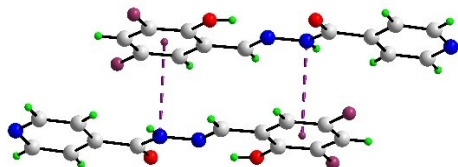
P. Yang, H. Chen, Z.-Z. Wang, L.-L. Zhang, D.-D. Zhang, Q.-S. Shi and X.-B. Xie, *J. Inorg. Biochem.*, 2020, **213**, 111248, <https://doi.org/10.1016/j.jinorgbio.2020.111248>



$d(\text{HN}\cdots\text{Cg}) = 3.31 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.58 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.23 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 14.0^\circ$;
sum of angles about $\text{N}(\text{H}) = 360.0^\circ$

a24. PEPDIA $(\text{E})\text{-N}'\text{-}(3,5\text{-difluoro-2-hydroxybenzylidene})\text{isonicotinohydrazide}$

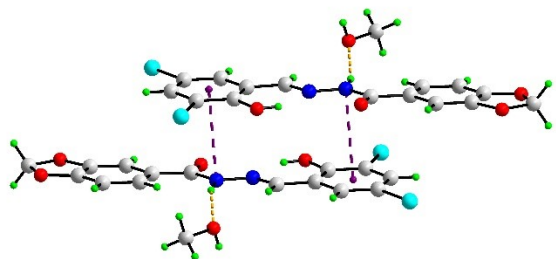
S. Mittapalli, D. S. Perumalla, J. B. Nanubolu and A. Nangia, *IUCrJ*, 2017, **4**, 812-823, <https://doi.org/10.1107/S2052252517014658>



$d(\text{HN}\cdots\text{Cg}) = 3.39 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.32 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.39 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 2.3^\circ$;
sum of angles about $\text{N}(\text{H}) = 360.0^\circ$

a25. QOTWUS $\text{N}'\text{-}(3,5\text{-dichloro-2-hydroxybenzylidene})\text{-1,3-benzodioxole-5-carbohydrazide}$
methanol solvate

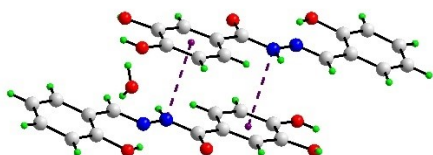
D.-X. Wu, J. Sun and M.-Z. Huang, *Z. Kristallogr. - New Cryst. Struct.*, 2009, **224**, 227-228, <https://doi.org/10.1524/ncrs.2009.0101>



$d(\text{HN}\cdots\text{Cg}) = 3.38 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.44 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.36 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 3.7^\circ$;
sum of angles about $\text{N}(\text{H}) = 359.4^\circ$

a26. RITFIK 3,4-dihydroxy- N' -(2-hydroxybenzylidene)benzohydrazide methanol solvate sesquihydrate

H.-B. Ma, S.-S. Huang and Y.-P. Diao, *Acta Crystallogr., Sect. E: Cryst. Commun.*, 2008, **64**, o210, <https://doi.org/10.1107/S1600536807065038>

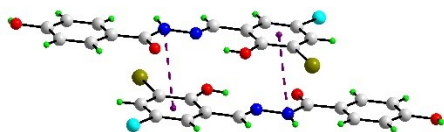


Two independent molecules – one self-associates into a dimer

$d(\text{HN}\cdots\text{Cg}) = 3.37 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.45 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.39 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 3.7^\circ$;
sum of angles about $\text{N}(\text{H}) = 359.9^\circ$

a27. ROFMOP N' -(3-bromo-5-chloro-2-hydroxybenzylidene)-4-hydroxybenzohydrazide

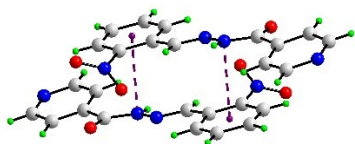
L.-W. Xue, Y.-J. Han, C.-J. Hao, G.-Q. Zhao and Q.-R. Liu, *Acta Crystallogr., Sect. E: Cryst. Commun.*, 2008, **64**, o1938, <https://doi.org/10.1107/S160053680802905X>



$d(\text{HN}\cdots\text{Cg}) = 3.44 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.40 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.46 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 1.5^\circ$;
sum of angles about $\text{N}(\text{H}) = 359.7^\circ$

a28. TIMZAQ03 2-nitrobenzaldehyde isonicotinoylhydrazone

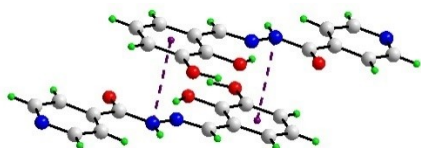
S. M. S. V. Wardell, M. V. N. de Souza, J. L. Wardell, J. N. Low and C. Glidewell, *Acta Crystallogr., Sect. C: Struct. Chem.*, 2005, **61**, o683-o689, <https://doi.org/10.1107/S0108270105032580>



$d(\text{HN}\cdots\text{Cg}) = 3.42 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.23 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.37 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 8.8^\circ$;
sum of angles about $\text{N}(\text{H}) = 359.9^\circ$

a29. WAFVEG N' -(2,3-dihydroxybenzylidene)isonicotinohydrazide

E. Tecer, N. Dege, A. Zülfiyaroglu, N. Senyüz and H. Batil, *Acta Crystallogr., Sect. E: Cryst. Commun.*, 2010, **66**, o3369-o3370, <https://doi.org/10.1107/S1600536810048701>

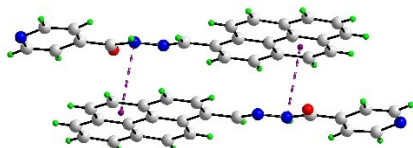


Two independent molecules, only one forms an interaction

$d(\text{HN}\cdots\text{Cg}) = 3.39 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.42 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.39 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 1.3^\circ$;
sum of angles about $\text{N}(\text{H}) = 359.9^\circ$

a30. WOTZEN N' -[(pyren-1-yl)methylidene]pyridine-4-carbohydrazide methanol solvate

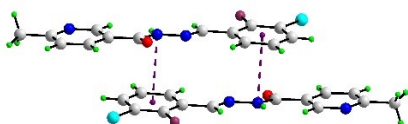
L. Wang, *Z. Kristallogr. - New Cryst. Struct.*, 2019, **234**, 1249-1250, <https://doi.org/10.1515/ncrs-2019-0370>



$d(\text{HN}\cdots\text{Cg}) = 3.37 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.51 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.45 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 9.8^\circ$;
sum of angles about $\text{N}(\text{H}) = 360.0^\circ$

a31. XAZXON N' -[(E)-3-chloro-2-fluorobenzylidene]-6-methylnicotinohydrazide monohydrate

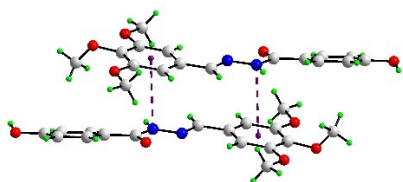
H.-K. Fun, C. K. Quah, P. C. Shyma, B. Kalluraya and J. H. S. Vidyashree, *Acta Crystallogr., Sect. E: Cryst. Commun.*, 2012, **68**, o2122, <https://doi.org/10.1107/S1600536812026736>



$d(\text{HN}\cdots\text{Cg}) = 3.36 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.51 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.45 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 10.6^\circ$;
sum of angles about $\text{N}(\text{H}) = 360.0^\circ$

a32. YAGYAI (E)-4-hydroxy-N'-(3,4,5-trimethoxybenzylidene)benzohydrazide

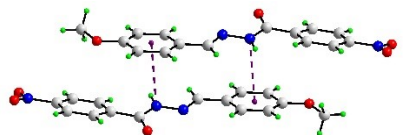
J. Horkaew, S. Chantrapromma and H.-K. Fun, *Acta Crystallogr., Sect. E: Cryst. Commun.*, 2011, **67**, o2985, <https://doi.org/10.1107/S1600536811041535>



$d(\text{HN}\cdots\text{Cg}) = 3.45 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.44 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.37 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 8.5^\circ$;
sum of angles about N(H) = 360.0°

a33. YIXNID N'-(4-methoxybenzylidene)-4-nitrobenzohydrazide methanol solvate

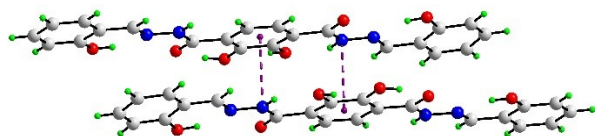
Y.-Z. Wang, M.-D. Wang, Y.-P. Diao and Q. Cai, *Acta Crystallogr., Sect. E: Cryst. Commun.*, 2008, **64**, o668, <https://doi.org/10.1107/S1600536808005813>



$d(\text{HN}\cdots\text{Cg}) = 3.40 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.62 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.47 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 13.3^\circ$;
sum of angles about N(H) = 360.0°

a34. GINPOL 2,3-dihydroxy-N',N'-bis[(2-hydroxyphenyl)methylidene]benzene-1,4-dicarbohydrazide

T. Kundu, J. Wang, Y. Cheng, Y. Du, Y. Qian, G. Liu and D. Zhao, *Dalton Trans.*, 2018, **47**, 13824-13829, <https://doi.org/10.1039/C8DT03005G>



Two residues

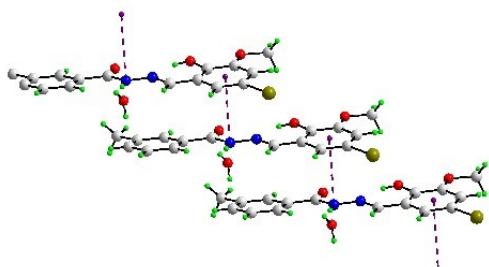
$d(\text{HN}\cdots\text{Cg}) = 3.33 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.39 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.33 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 2.1^\circ$;
sum of angles about N(H) = 360.0°

Linear chain:

a35. AVEZUY N'-(5-bromo-2-hydroxy-3-methoxybenzylidene)-3-methylbenzohydrazide monohydrate

W.-M. Zhang, G.-H. Sheng and Z. You, *Asian J. Chem.*, 2014, **26**, 8118-8122,

<https://doi.org/10.14233/ajchem.2014.17602>

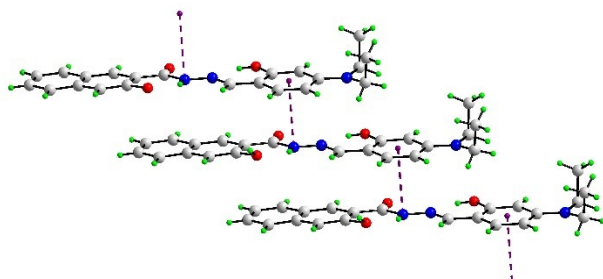


$d(\text{HN}\cdots\text{Cg}) = 3.42 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.55 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.43 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 6.4^\circ$;
sum of angles about N(H) = 360.0°

a36. BESH0Z N'-[[4-(diethylamino)-2-hydroxyphenyl]methylidene]-3-hydroxynaphthalene-2-carbohydrazide

M. Wu, D. Wang, J.-Q. Zheng, D.-C. Fang, L.-P. Jin and X.-J. Zheng, *Chem. Sel.*, 2018, **3**, 2174-2180,

<https://doi.org/10.1002/slct.201702611>

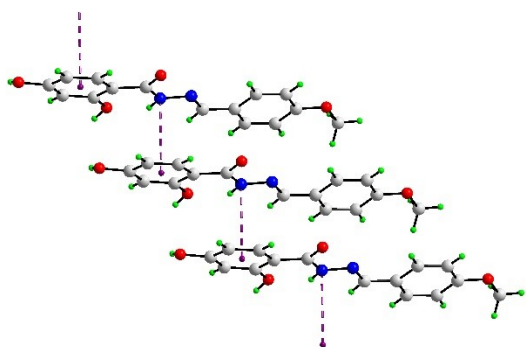


$d(\text{HN}\cdots\text{Cg}) = 3.35 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.40 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.42 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 5.7^\circ$;
sum of angles about N(H) = 360.0°

a37. GITBAN trans-2,4-dihydroxy-N'-(4-methoxybenzylidene)benzohydrazide

Y.-P. Diao, S.-S. Huang, J.-K. Zhang and T.-G. Kang, *Acta Crystallogr., Sect. E: Cryst. Commun.*, 2008, **64**,

o470, <https://doi.org/10.1107/S1600536808001104>

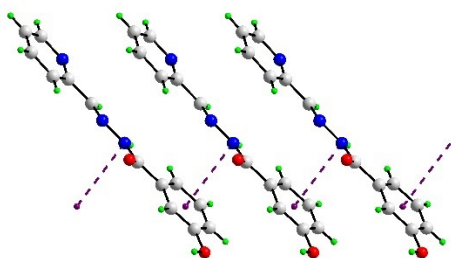


$d(\text{HN}\cdots\text{Cg}) = 3.43 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.54 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.59 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 9.5^\circ$;
sum of angles about $\text{N}(\text{H}) = 360.0^\circ$

a38. HIGCUW 2-pyridinecarbaldehyde-3'-hydroxybenzoyl hydrazone

P. V. Bernhardt, P. Chin, P. C. Sharpe and D. R. Richardson, *Dalton Trans.*, 2007, 3232-3244,

<https://doi.org/10.1039/b704102k>

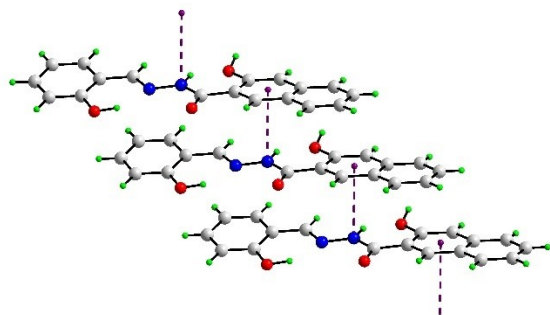


$d(\text{HN}\cdots\text{Cg}) = 3.37 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.57 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.43 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 13.3^\circ$;
sum of angles about $\text{N}(\text{H}) = 360.0^\circ$

a39. HUGPOP (E)-3-hydroxy-N'-(2-hydroxybenzylidene)-2-naphthohydrazide

H. H. Monfared, R. Bikas and P. Mayer, *Acta Crystallogr., Sect. E: Cryst. Commun.*, 2010, **66**, o236-o237,

<https://doi.org/10.1107/S1600536809053793>

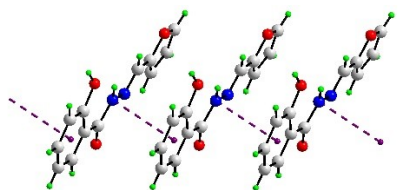


$d(\text{HN}\cdots\text{Cg}) = 3.30 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.42 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.39 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 7.3^\circ$;
sum of angles about $\text{N}(\text{H}) = 360.0^\circ$

a40. IGAJOQ N'-(2-furylmethylene)-2-hydroxybenzohydrazide

Y.-X. Zhang, *Acta Crystallogr., Sect. E: Cryst. Commun.*, 2008, **64**, o2208,

<https://doi.org/10.1107/S1600536808034636>



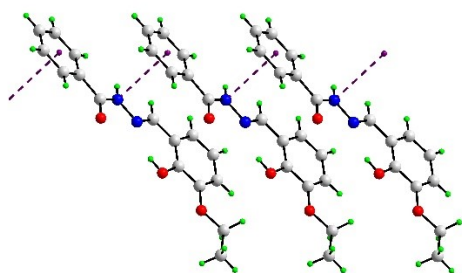
$d(\text{HN}\cdots\text{Cg}) = 3.41 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.53 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.44 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 5.6^\circ$;

sum of angles about N(H) = 360.0°

a41. JOFXOU N'-[(3-ethoxy-2-hydroxyphenyl)methylidene]benzohydrazide monohydrate

M. C. Vineetha, M. Sithambaresan, Y. S. Nair, M. R. Prathapachandra Kurup, *Inorg. Chim. Acta*, 2019,

419, 93-104, <https://doi.org/10.1016/j.ica.2019.03.040>



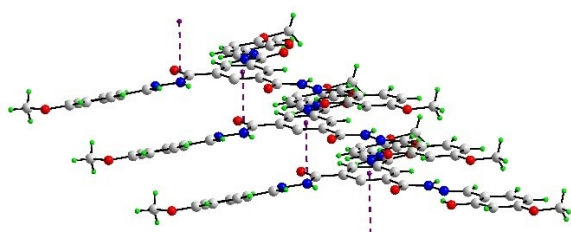
$d(\text{HN}\cdots\text{Cg}) = 3.43 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.86 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.77 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 7.7^\circ$;

sum of angles about N(H) = 360.0°

a42. JUQLOZ N'1,N'3,N'5-tris[(2-hydroxy-4-methoxyphenyl)methylidene]benzene-1,3,5-tricarbohydrazide N,N-dimethylformamide solvate

P. Muthukumar, M. Surya, M. Pannipara, A. G. Al-Sehemi, D. Moon and S. P. Anthony, *Chem. Sel.*,

2020, **5**, 3295-3302, <https://doi.org/10.1002/slct.201904875>

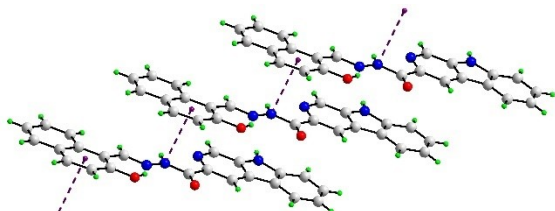


$d(\text{HN}\cdots\text{Cg}) = 3.33 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.30 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.48 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 3.4^\circ$;

sum of angles about N(H) = 359.6°

a43. KENNUO N'-((2-hydroxy-1-naphthyl)methylene)-9H-b-carboline-3-carbohydrazide monohydrate

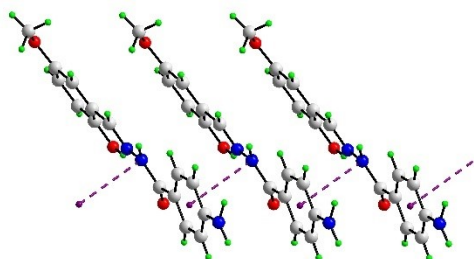
Y.-F. Sun, Z.-Y. Chen, Y.-L. Liu, N. Li, J.-K. Li and H.-C. Song, *Dyes Pigm.*, 2012, **95**, 512-522, <https://doi.org/10.1016/j.dyepig.2012.06.002>



$d(\text{HN}\cdots\text{Cg}) = 3.44 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.53 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.43 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 4.0^\circ$;
sum of angles about N(H) = 360.0°

a44. LEDVUN N'-((2-hydroxy-1-naphthyl)methylene)-9H-b-carboline-3-carbohydrazide monohydrate

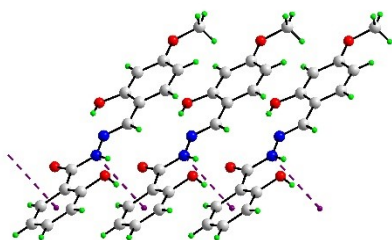
H. Kargar, R. Kia and M. N. Tahir, *Acta Crystallogr., Sect. E: Cryst. Commun.*, 2012, **68**, o2321-o2322, <https://doi.org/10.1107/S1600536812026633>



$d(\text{HN}\cdots\text{Cg}) = 3.42 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.77 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.46 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 17.7^\circ$;
sum of angles about N(H) = 359.9°

a45. LUGXOD (E)-N'-(2-hydroxy-4-methoxybenzylidene)-2-hydroxybenzohydrazide

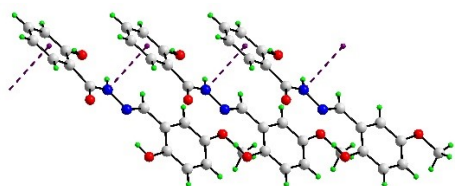
P. Muthukumar, M. Surya, M. Pannipara, A. G. Al-Sehemi, D. Moon, S. P. Anthony, *Chem. Sel.*, 2020, **5**, 3295-3302, <https://doi.org/10.1002/slct.201904875>



$d(\text{HN}\cdots\text{Cg}) = 3.45 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.55 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.55 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 8.4^\circ$;
sum of angles about N(H) = 360.0°

a46. LUGXUJ (E)-N'-(2-hydroxy-5-methoxybenzylidene)-2-hydroxybenzohydrazide

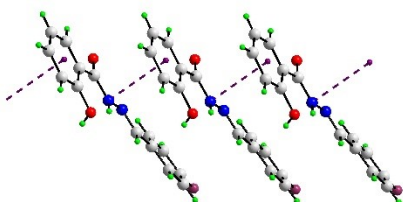
P. Muthukumar, M. Surya, M. Pannipara, A. G. Al-Sehemi, D. Moon, S. P. Anthony, *Chem. Sel.*, 2020, **5**, 3295-3302, <https://doi.org/10.1002/slct.201904875>



$d(\text{HN}\cdots\text{Cg}) = 3.39 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.53 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.48 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 9.0^\circ$;
sum of angles about N(H) = 360.0°

a47. MEBLIP 4-fluorobenzaldehyde (2-hydroxybenzoyl)hydrazone

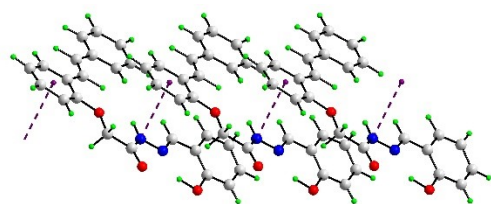
Y. Zhang, S.-P. Zhang, Y.-Y. Wu and S.-C. Shao, *Acta Crystallogr., Sect. E: Cryst. Commun.*, 2006, **62**, o119-o120, <https://doi.org/10.1107/S1600536805040420>



$d(\text{HN}\cdots\text{Cg}) = 3.39 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.48 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.46 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 5.1^\circ$;
sum of angles about N(H) = 360.0°

a48. OCANOV N-(E)-(2-stilbenyloxyacetyl) o-hydroxybenzaldehyde hydrazone

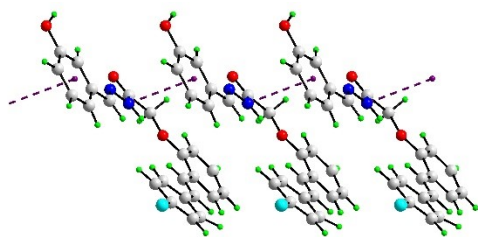
E. Wyrzykiewicz, A. Błaszczyk and I. Turowska-Tyrk, *Bull. Pol. Acad. Sci., Chem.*, 2000, **48**, 212-229.



$d(\text{HN}\cdots\text{Cg}) = 3.36 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.60 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.39 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 9.4^\circ$;
sum of angles about N(H) = 359.5°

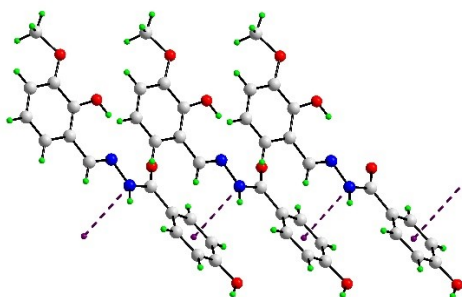
a49. OCANUB N-(E)-(2-(4'-chlorostilbenyl)oxyacetyl) m-hydroxybenzaldehyde hydrazone

E. Wyrzykiewicz, A. Błaszczyk and I. Turowska-Tyrk, *Bull. Pol. Acad. Sci., Chem.*, 2000, **48**, 212-229.



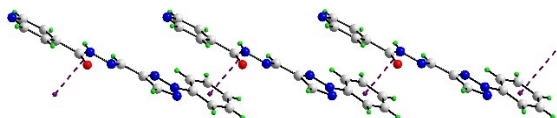
$d(\text{HN}\cdots\text{Cg}) = 3.38 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.68 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.45 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 17.3^\circ$;
sum of angles about $\text{N}(\text{H}) = 360.0^\circ$

a50. ROGFEZ01 4-hydroxy- N' -(2-hydroxy-3-methoxybenzylidene)benzohydrazide monohydrate
J. N. Low and J. L. Wardell, Private Communication to the Cambridge Structural Database, Refcode
ROGFEZ01, 2018.



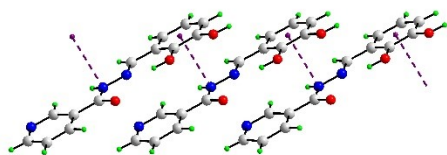
$d(\text{HN}\cdots\text{Cg}) = 3.44 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.71 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.65 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 15.1^\circ$;
sum of angles about $\text{N}(\text{H}) = 359.0^\circ$

a51. WIWGOB N' -[(2-phenyl-2H-1,2,3-triazol-4-yl)methylidene]pyridine-4-carbohydrazide dihydrate
D. T. G. Gonzaga, F. C. da Silva, V. F. Ferreira, J. L. Wardell and S. M. S. V. Wardell, *J. Braz. Chem. Soc.*,
2016, **27**, 2322-2333, <https://doi.org/10.5935/0103-5053.20160129>



$d(\text{HN}\cdots\text{Cg}) = 3.36 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.54 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.37 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 3.7^\circ$;
sum of angles about $\text{N}(\text{H}) = 359.9^\circ$

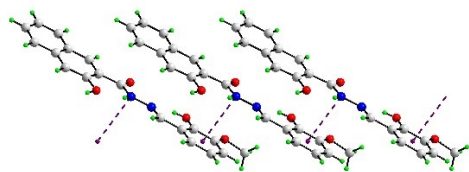
a52. WOFYUN N' -[(4-methoxyphenyl)methylidene]-2-(5-phenyl-2H-tetrazol-2-yl)acetohydrazide
N. Dege, N. Şenyüz, H. Bati, N. Günay, D. Avcı, Ö. Tamer and Y. Atalay, *Spectrochim. Acta Part A Mol. Biomol.*, 2014, **120**, 323-331, <https://doi.org/10.1016/j.saa.2013.10.030>



$d(\text{HN}\cdots\text{Cg}) = 3.39 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.35 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.49 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 4.6^\circ$;
sum of angles about $\text{N}(\text{H}) = 359.7^\circ$

a53. WUQYEP 3-hydroxy-*N'*-[(2-hydroxy-3-methoxyphenyl)methylidene]naphthalene-2-carbohydrazide

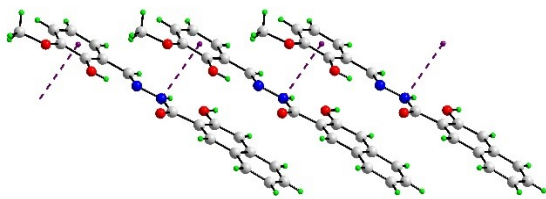
U. Saha, B. Das, M. Dolai, R. J. Butcher and G. S. Kumar, *ACS Omega*, 2020, **5**, 18411-18423,
<https://doi.org/10.1021/acsomega.0c02226>



$d(\text{HN}\cdots\text{Cg}) = 3.40 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.37 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.43 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 1.7^\circ$;
sum of angles about $\text{N}(\text{H}) = 360.0^\circ$

a54. WUQYEP01 3-hydroxy-*N'*-[(2-hydroxy-3-methoxyphenyl)methylidene]naphthalene-2-carbohydrazide

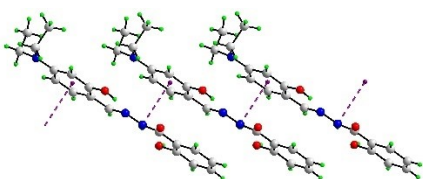
M. W., D.-D. Yang, H.-W. Zheng, Q.-F. Liang, J.-B. Li, Y. Kang, S. Li, C. Jiao, X.-J. Zheng and L.-P. Jin,
Dalton Trans, 2021, **50**, 1507-1513, <https://doi.org/10.1039/D0DT04062B>



$d(\text{HN}\cdots\text{Cg}) = 3.36 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.28 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.41 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 2.5^\circ$;
sum of angles about $\text{N}(\text{H}) = 360.0^\circ$

a55. ZOJSAV *N'*-[[4-(diethylamino)-2-hydroxyphenyl]methylidene]-2-hydroxybenzohydrazide

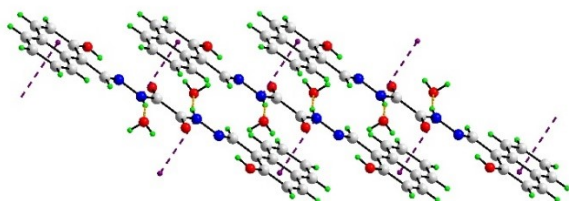
V. Felix, Private Communication to the Cambridge Structural Database, Refcode ZOJSAV, 2019.



$d(\text{HN}\cdots\text{Cg}) = 3.26 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.35 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.36 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 8.5^\circ$;
sum of angles about $\text{N}(\text{H}) = 360.0^\circ$

a56. NEQOOQ bis(2-hydroxy-1-naphthaldehyde) oxaloyldihydrazone dihydrate

L.-N. Zhu, C.-Q. Li, X.-Z. Li and R. Li, *Acta Crystallogr., Sect. E: Cryst. Commun.*, 2006, **62**, o4603-o4605,
<https://doi.org/10.1107/S1600536806037615>

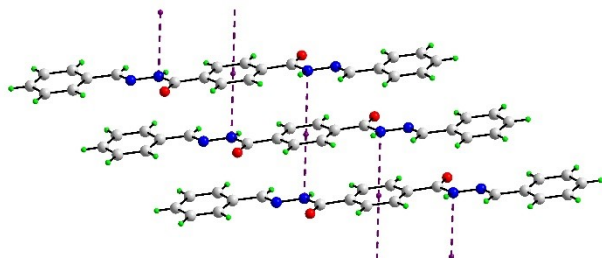


Centrosymmetric molecule: two interactions per molecule

$d(\text{HN}\cdots\text{Cg}) = 3.32 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.29 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.30 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 0.8^\circ$;
sum of angles about $\text{N}(\text{H}) = 360.0^\circ$

a57. IHIPEx N'1,N'4-dibenzylidenebenzene-1,4-dicarbohydrazide dihydrate

X. Li, J. Qiao, S. W. Chee, H.-S. Xu, X. Zhao, H. S. Choi, W. Yu, S. Y. Quek, U. Mirsaidov and K. P. Loh, *J. Am. Chem. Soc.*, 2020, **142**, 4932-4943, <https://doi.org/10.1021/jacs.0c00553>



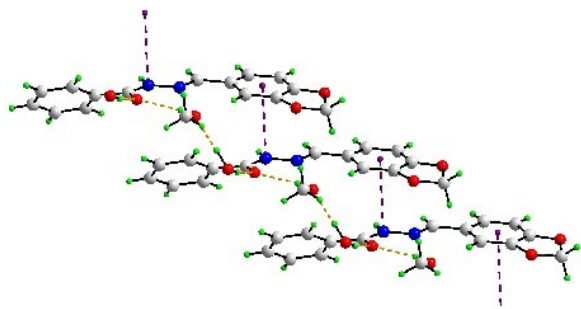
The molecule is centred around an inversion centre; each ring forms two contacts

$d(\text{HN}\cdots\text{Cg}) = 3.38 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.39 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.34 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 1.0^\circ$;
sum of angles about $\text{N}(\text{H}) = 359.4^\circ$

Linear chains also featuring conventional hydrogen bonding:

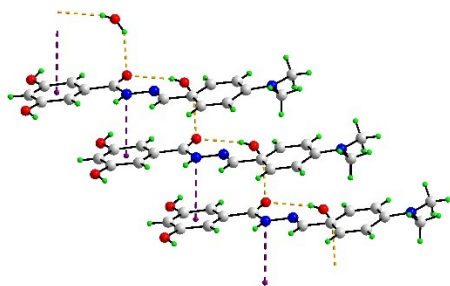
a58. BOLFUG N'-[(2H-1,3-benzodioxol-5-yl)methylidene]benzohydrazide methanol solvate monohydrate

V. Arumugam, C. Shalini, N. Dharmaraj, W. Kaminsky and R. Karvembu, *Eur. J. Inorg. Chem.*, 2019, 3869-3882, <https://doi.org/10.1002/ejic.201900781>



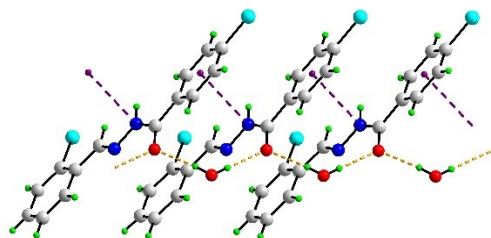
$d(\text{HN}\cdots\text{Cg}) = 3.40 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.44 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.28 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 8.0^\circ$;
sum of angles about $\text{N}(\text{H}) = 360.0^\circ$

a59. CIQVAA N'-(4-(dimethylamino)benzylidene)-3,5-dihydroxybenzohydrazide monohydrate
Y.-P. Diao, J.-K. Zhang, S.-Q. Xie and T.-G. Kang, *Acta Crystallogr., Sect. E: Cryst. Commun.*, 2007, **63**,
o4908, <https://doi.org/10.1107/S1600536807061132>



$d(\text{HN}\cdots\text{Cg}) = 3.38 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.50 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.39 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 4.6^\circ$;
sum of angles about $\text{N}(\text{H}) = 360.0^\circ$

a60. COGQEW (E)-4-chloro-N'-(2-chlorobenzylidene)benzohydrazide monohydrate
J. T. Mague, S. K. Mohamed, M. Akkurt, H. Potgieter and M. R. Albayati, *Acta Crystallogr., Sect. E:*
Cryst. Commun., 2014, **70**, o612, <https://doi.org/10.1107/S1600536814008885>

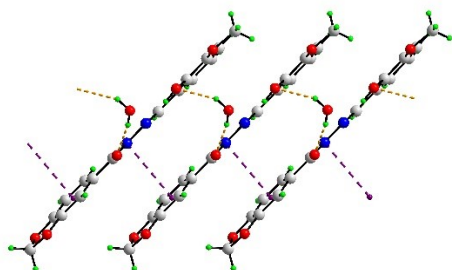


$d(\text{HN}\cdots\text{Cg}) = 3.44 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.75 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.43 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 14.7^\circ$;
sum of angles about $\text{N}(\text{H}) = 360.0^\circ$

a61. MOKHIE N'-(2-hydroxy-3-methoxybenzylidene)-1,3-benzodioxole-5-carbohydrazide monohydrate

C.-L. Du, *Acta Crystallogr., Sect. E: Cryst. Commun.*, 2009 **65**, o29,

<https://doi.org/10.1107/S1600536808040117>

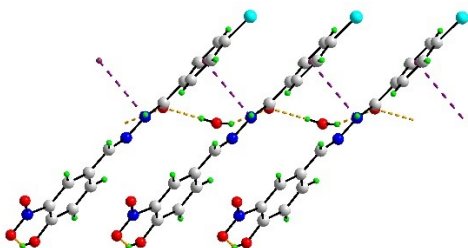


$d(\text{HN}\cdots\text{Cg}) = 3.45 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.59 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.47 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 7.4^\circ$;
sum of angles about N(H) = 360.0°

a62. QAPHAS 4-chloro-N'-(4-hydroxy-3-nitrobenzylidene)benzohydrazide monohydrate

Y. Lei, T.-Z. Li, C. Fu, X.-L. Guan and Y. Tan, *J. Chem. Crystallogr.*, 2011, **41**, 1707,

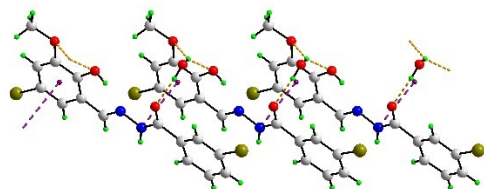
<https://doi.org/10.1007/s10870-011-0161-0>



$d(\text{HN}\cdots\text{Cg}) = 3.32 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.63 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.40 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 15.3^\circ$;
sum of angles about N(H) = 359.7°

a63. SEDTUS 3-bromo-N'-(5-bromo-2-hydroxy-3-methoxybenzylidene)benzohydrazide monohydrate

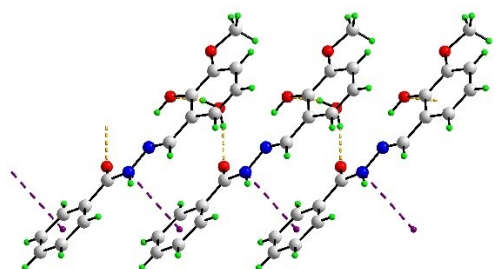
H.-Y. Zhu, *Asian J. Chem.*, 2012, **24**, 558-560.



$d(\text{HN}\cdots\text{Cg}) = 3.45 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.55 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.44 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 4.3^\circ$;
sum of angles about N(H) = 358.5°

a64. TEZMER N'-[(2-hydroxy-3-methoxyphenyl)methylidene]benzohydrazide monohydrate

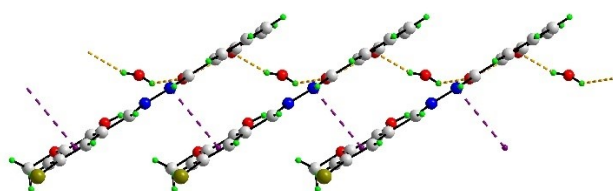
O. Pouralimardan, A.-C. Chamayou, C. Janiak and H. Hosseini-Monfared, *Inorg. Chim. Acta*, 2007, **360**, 1599-1608, <https://doi.org/10.1016/j.ica.2006.08.056>



$d(\text{HN}\cdots\text{Cg}) = 3.41 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.40 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.53 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 3.1^\circ$;
sum of angles about N(H) = 359.9°

a65. XAZHUD (E)-N'-(5-bromo-2-hydroxy-3-methoxybenzylidene)-2-hydroxybenzohydrazide monohydrate

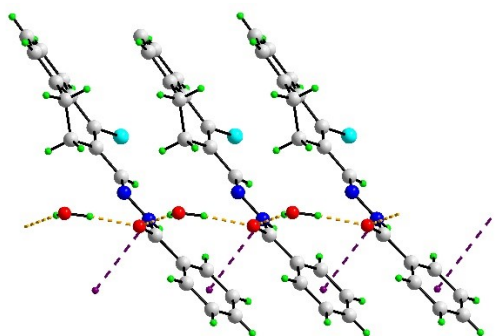
S. Zhao, L. Li, X. Liu, W. Feng and X. Lu, *Acta Crystallogr., Sect. E: Cryst. Commun.*, 2012, **68**, o2040, <https://doi.org/10.1107/S1600536812024816>



$d(\text{HN}\cdots\text{Cg}) = 3.42 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.35 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.42 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 4.6^\circ$;
sum of angles about N(H) = 360.0°

a66. ZOZMAF N'-[(1-chloro-3,4-dihydronaphthalen-2-yl)methylidene]benzohydrazide monohydrate

H. A. Arjun, G. N. Anil Kumar, R. Elancheran and S. Kabilan, *Acta Crystallogr., Sect. E: Cryst. Commun.*, 2020, **76**, 132-136, <https://doi.org/10.1107/S1600536808005813>

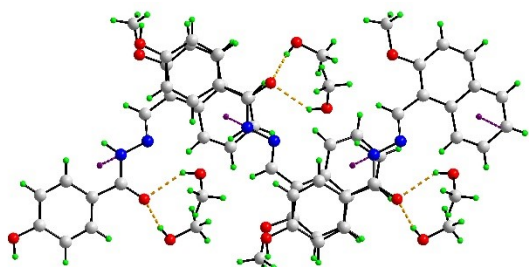


$d(\text{HN}\cdots\text{Cg}) = 3.43 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.64 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.50 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 11.1^\circ$;
sum of angles about N(H) = 359.7°

Zigzag chain:

a67. GEKCOQ 4-hydroxy-N'-((2-methoxy-1-naphthyl)methylidene)benzohydrazide methanol solvate

Y.-J. Wei and E.-W. Wang, *J. Struct. Chem.*, 2011, **52**, 775, <https://doi.org/10.1134/S0022476611040160>



$d(\text{HN}\cdots\text{Cg}) = 3.43 \text{ \AA}$; $\text{C}\cdots\text{C} = 3.59 \text{ \AA}$; $\text{N}\cdots\text{C} = 3.56 \text{ \AA}$; dihedral angle $\text{C}_2\text{N}_2\text{O}/\text{C}_6 = 11.5^\circ$;

sum of angles about $\text{N}(\text{H}) = 359.8^\circ$