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Dominant role of C-Br···N halogen bond in molecular self-organization. Crystallographic and quantum-chemical study of Schiff-base-containing triazoles.

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Three Schiff-base-containing triazole derivatives have been synthesized and investigated by X-ray crystallography. Structural motifs (*zigzag* or linear chains) formed in the solid state are stabilized by C−Br···N halogen bond interactions, while hydrogen bonds do not seem to play a significant role in the molecular self-organization of studied compounds. Quantum-chemical studies confirm that these interactions are sufficient to account for both the arrangement of structural motifs and very short Br···N distances observed experimentally. It is also shown that Br···N interactions can lead to generally shorter donor−acceptor distances than Cl···N contacts.

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