Supporting Data for *Persistence of the self-complementary N-H···N tape motif in chloro-s-triazine crystals; crystal structures of the simazine and atrazine herbicides, their polymorphic and inclusion behaviour.*

Contents:

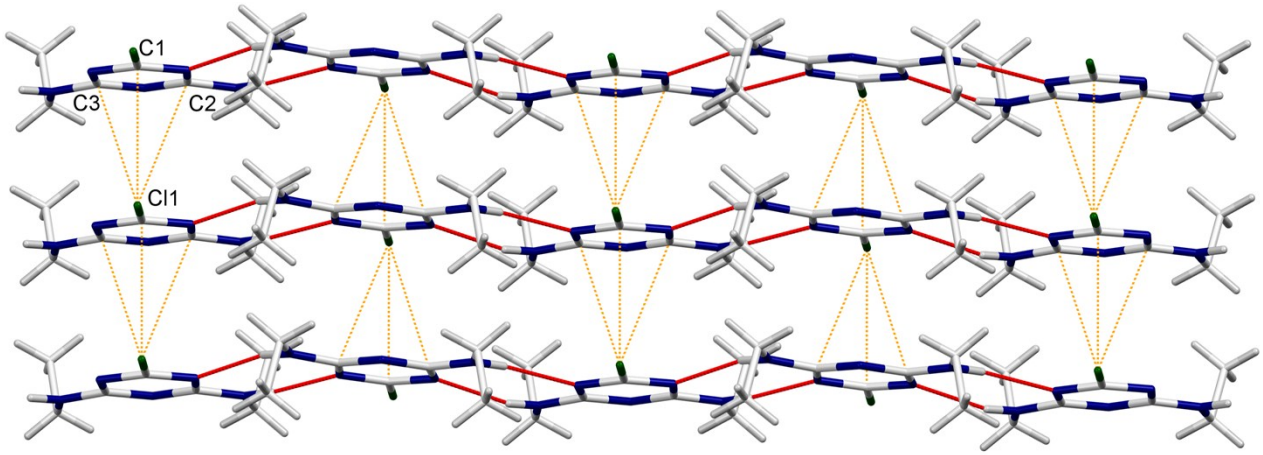
Three figures are presented the interactions occurring between self-complementary hydrogen-bonded tapes (S1-S3) and to visualise the isostructural character of $\mathbf{2}_{\text{Form\_II}}$ and **3** (S4).

Figure S1. Inter-tape packing of (a) **1**, and (b) $\mathbf{2}_{\text{Form\_I}}$ showing side chain interactions.

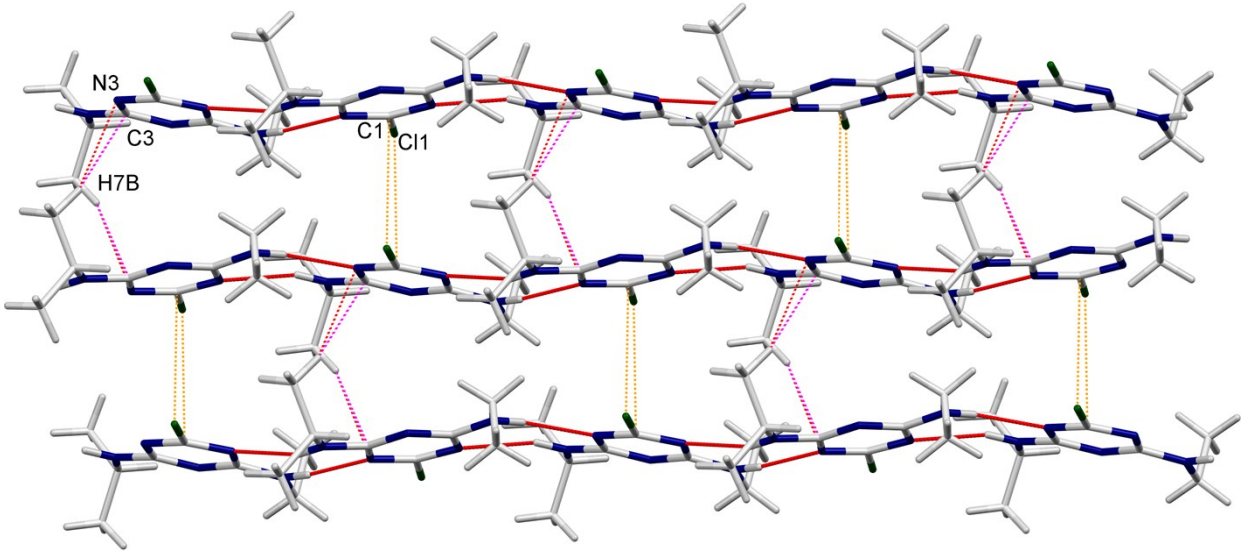
Figure S2. Inter-tape packing of (a) $\mathbf{2}_{\text{Form\_II}}$ and (b) **2.TCE** showing side chain interactions.

Figure S3: Packing of N-H···N tapes in (a) $\mathbf{1}_{\text{Form\_I}}$, and (b) $\mathbf{2}_{\text{Form\_I}}$. showing aromatic C···C interactions.

Figure S4: Packing in (a) $\mathbf{2}_{\text{Form\_II}}$ and (b) **3** indicating how these two structures are isostructural, despite the differences in space group.

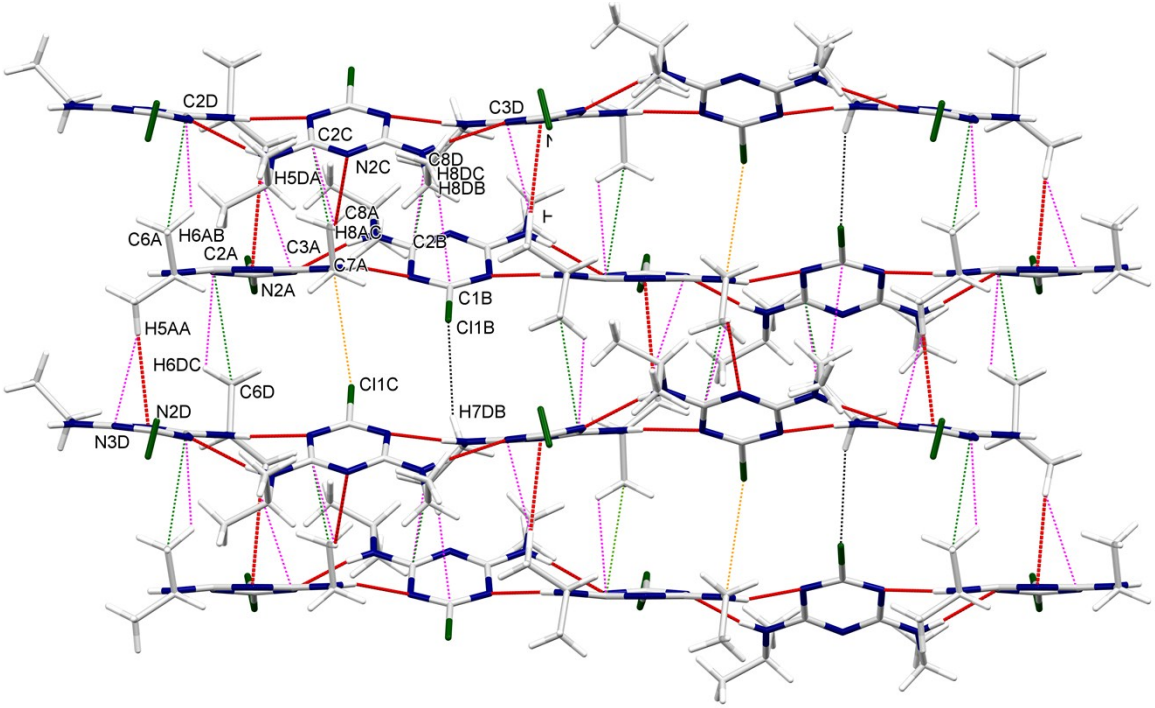


(a)

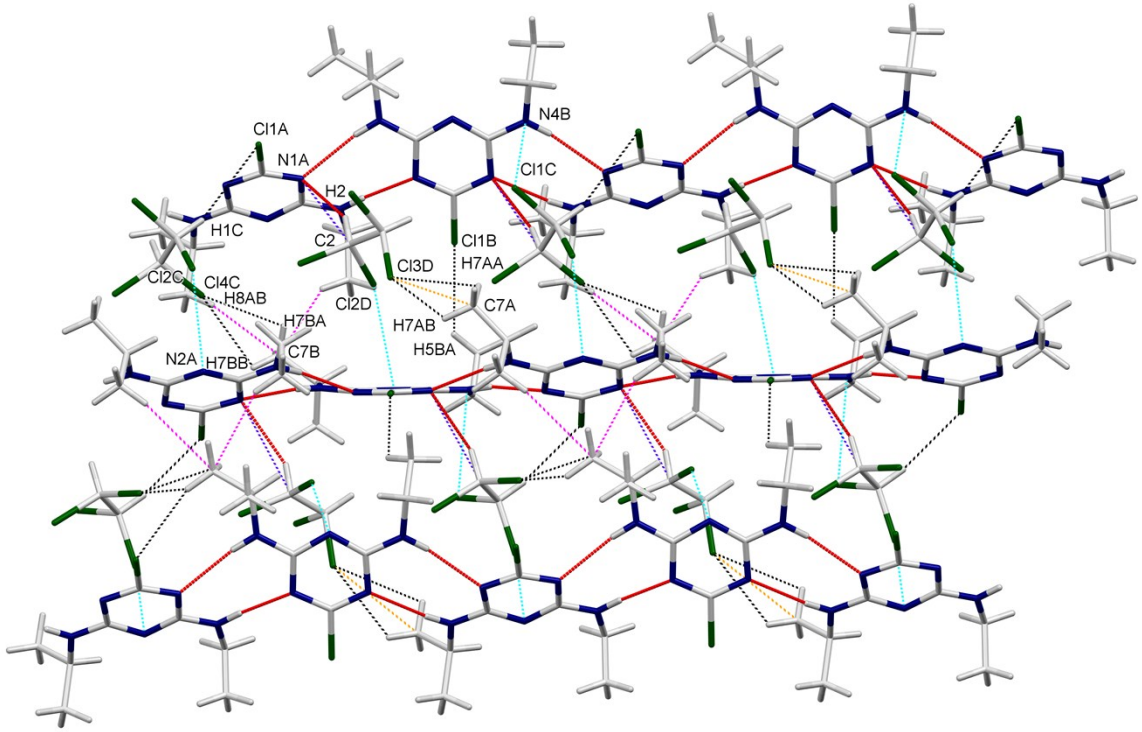


(b)

Figure S1. Inter-tape packing of (a) **1**, and (b) $\mathbf{2}_{\text{Form\_I}}$ showing side chain interactions. Interactions between the tapes are indicated as follows: N-H···N contacts are depicted in red, H···Cl contacts in black, Cl···π in orange, C-H···π in magenta, C···C in green N···Cl in light blue and C···N in purple.

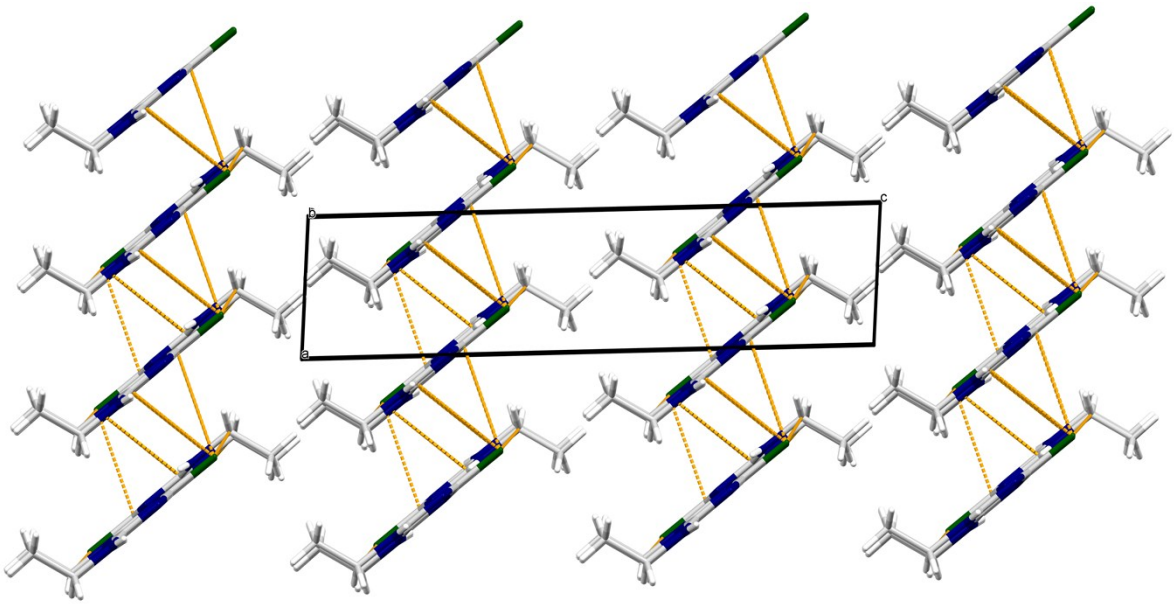


(a)

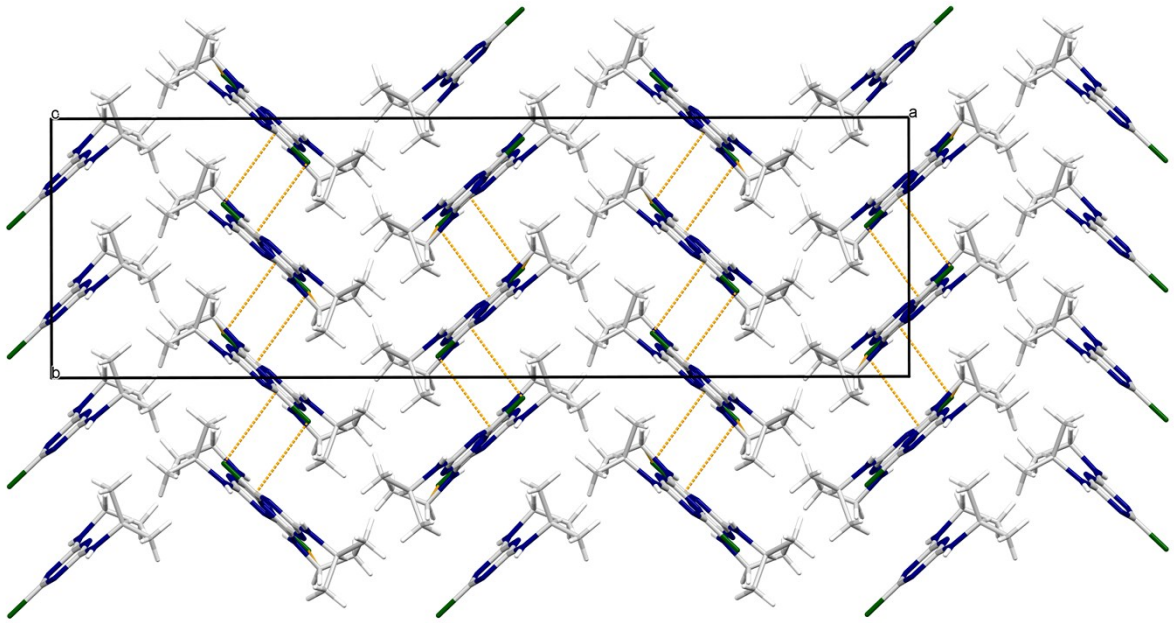


(b)

Figure S2. Inter-tape packing of (a) $\mathbf{2}_{\text{Form\_II}}$ and (b) **2.TCE** showing side chain interactions. Interactions between the tapes are indicated as follows: N-H···N contacts are depicted in red, H···Cl contacts in black, Cl···π in orange, C-H···π in magenta, C···C in green N···Cl in light blue and C···N in purple.

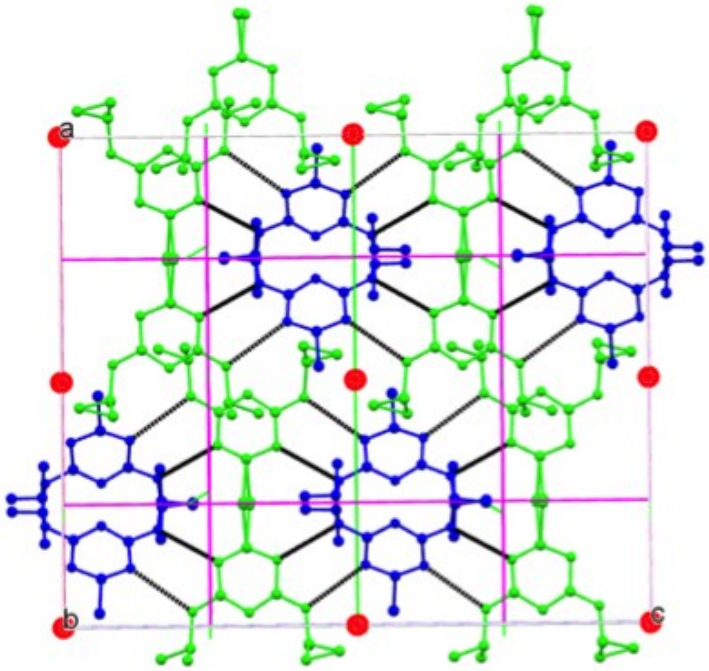


(a)

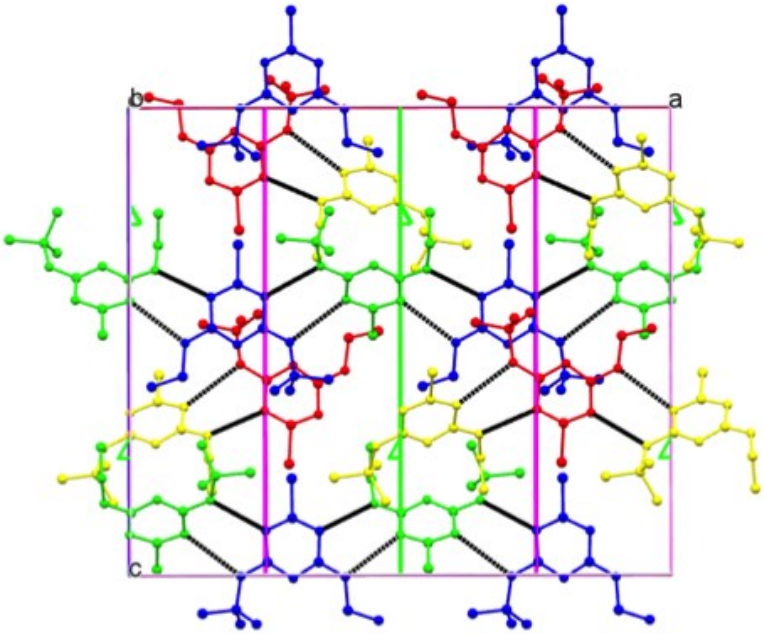


(b)

Figure S3: Packing of N-H···N tapes in (a) $\mathbf{1}_{\text{Form\_I}}$, and (b) $\mathbf{2}_{\text{Form\_I}}$. showing aromatic C···C interactions. Interactions are indicated by broken yellow lines.



(a)



(b)

Figure S4: Packing in (a) $\mathbf{2}_{\text{Form\_II}}$ and (b) **3** indicating how these two structures are isostructural, despite the differences in space group.