

Electronic Supplementary Information

Analysis of short contacts in crystals of halogenated amino acids: atom-atom interactions vs. energy frameworks

Francois J. De Beer, Fredrick J. F. Jacobs, Akho Ntsila, Dumisani V. Kama,* Vladimir A. Azov*

Department of Chemistry, University of the Free State, P.O. Box 339, 9300 Bloemfontein, South Africa.

* Corresponding author, email: azovv@ufs.ac.za, kamadv@ufs.ac.za

Table of Contents

Hirshfeld surface of Boc-Ala(3-Cl)-OMe (1)	2
Fingerprint plot of Boc-Ala(3-Cl)-OMe (1)	2
Hirshfeld surface of Boc-Ala(3-Cl)-O ^t Bu (2)	3
Fingerprint plot of Boc-Ala(3-Cl)-O ^t Bu (2)	3
Hirshfeld surface of Boc-Ala(3-Cl)-OBn (3)	4
Fingerprint plot of Boc-Ala(3-Cl)-OBn (3)	4
Hirshfeld surface of Fmoc-Ala(3-Cl)-O ^t Bu (4)	5
Fingerprint plot of Fmoc-Ala(3-Cl)-O ^t Bu (4)	5
Hirshfeld surface of Boc-Ala(3-I)-OMe (5)	6
Fingerprint plot of Boc-Ala(3-I)-OMe (5)	6
Hirshfeld surface of Boc-Ala(3-I)-O ^t Bu (6)	7
Fingerprint plot of Boc-Ala(3-I)-O ^t Bu (6)	7
Hirshfeld surface of Boc-Ala(3-I)-OBn (7)	8
Fingerprint plot of Boc-Ala(3-I)-OBn (7)	8
Hirshfeld surface of Fmoc-Ala(3-I)-O ^t Bu (8)	9
Fingerprint plot of Fmoc-Ala(3-I)-O ^t Bu (8)	9
NMR characterization of Boc-Ala(3-Cl)-O ^t Bu (2)	10
NMR characterization of Boc-Ala(3-Cl)-OBn (3)	11

Hirshfeld surface of Boc-Ala(3-Cl)-OMe (**1**)

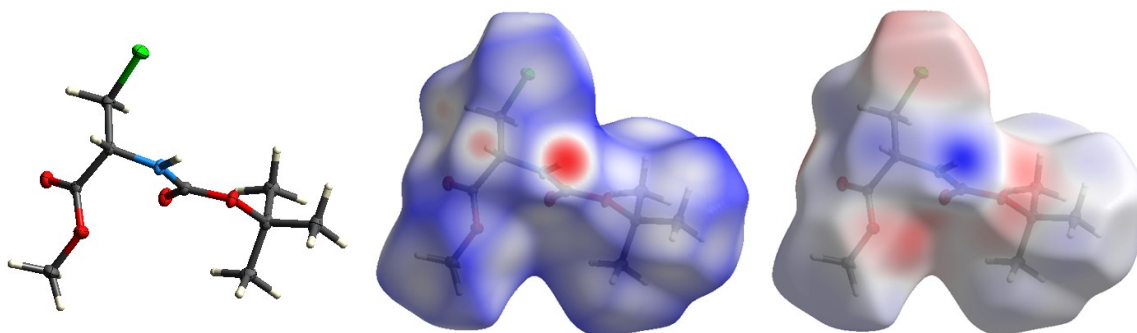


Figure S1. Molecular structure of **1** (left) and its Hirshfeld surface mapped with d_{norm} (middle) and ESP (right).

Fingerprint plot of Boc-Ala(3-Cl)-OMe (**1**)

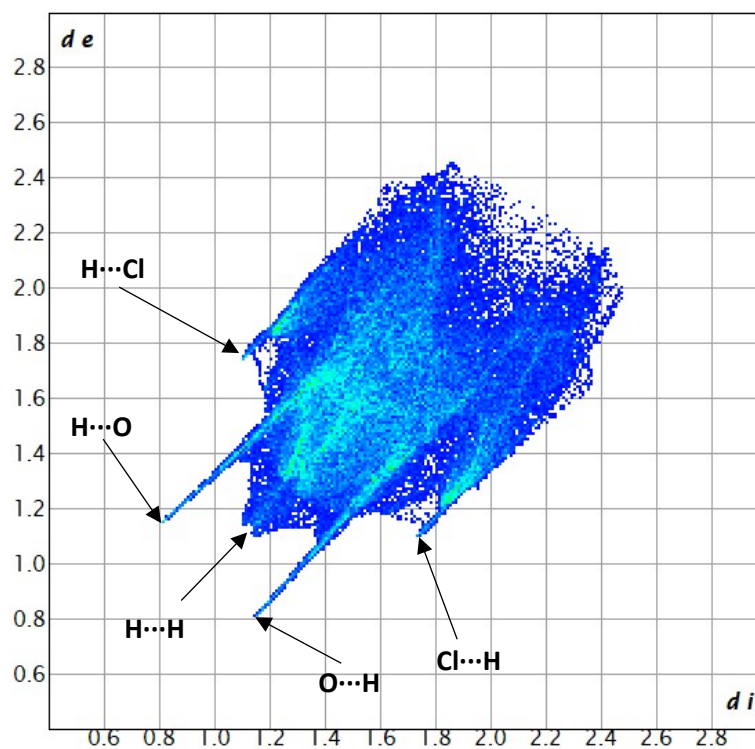


Figure S2. Fingerprint plot of **1**. Important intermolecular contacts are indicated with arrows.

Hirshfeld surface of Boc-Ala(3-Cl)-O^tBu (2)

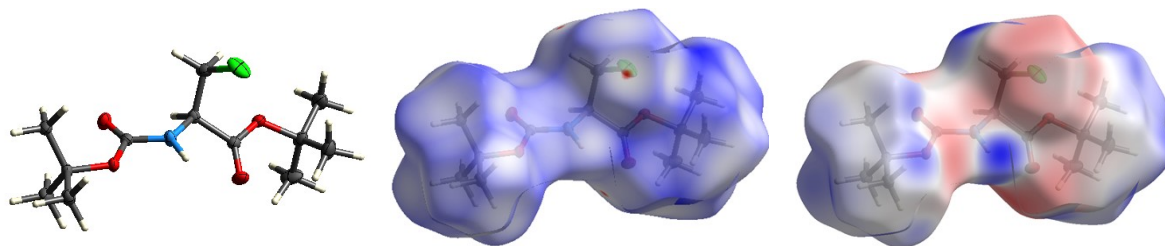


Figure S3. Molecular structure of **2** (left) and its Hirshfeld surface mapped with d_{norm} (middle) and ESP (right).

Fingerprint plot of Boc-Ala(3-Cl)-O^tBu (2)

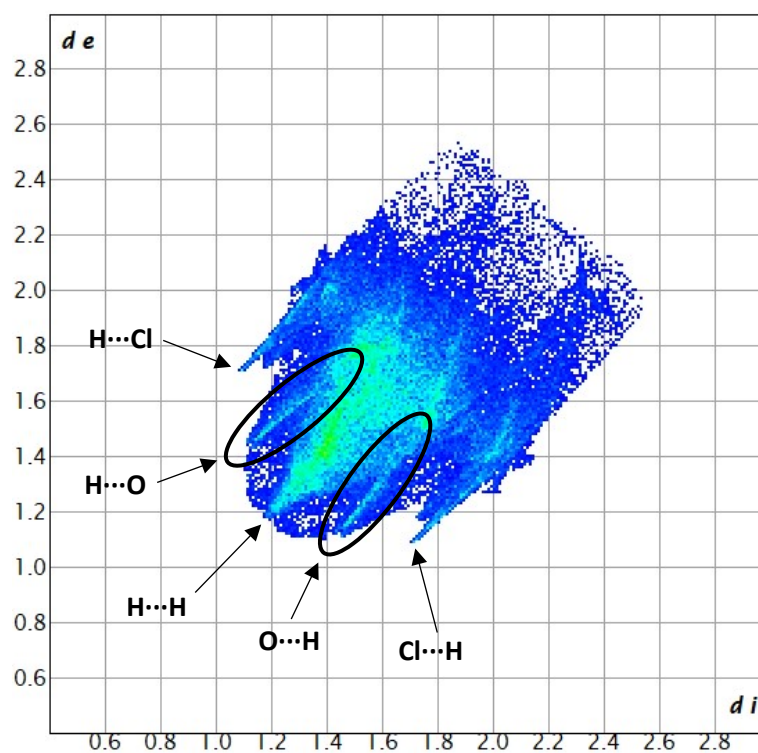


Figure S4. Fingerprint plot of **2**. Important intermolecular contacts are indicated with arrows.

Hirshfeld surface of Boc-Ala(3-Cl)-OBn (**3**)

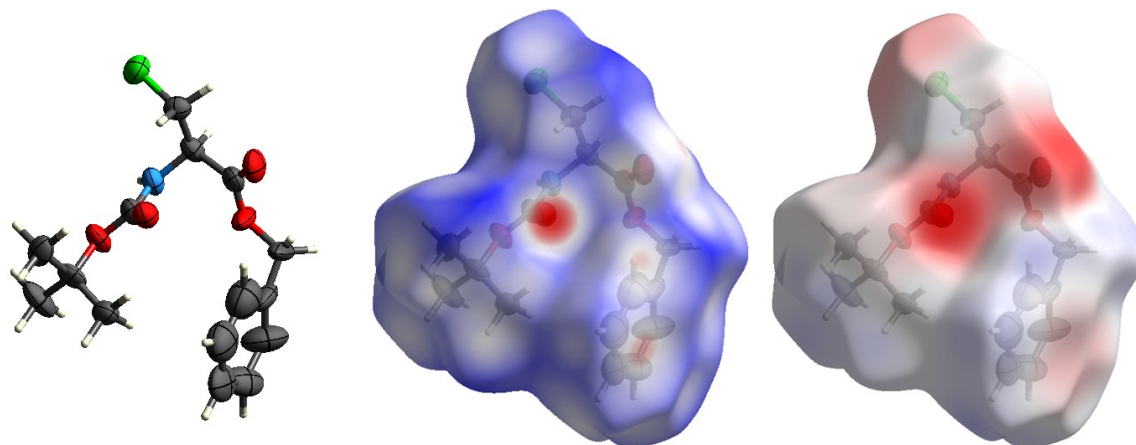


Figure S5. Molecular structure of **3** (left) and its Hirshfeld surface mapped with d_{norm} (middle) and ESP (right).

Fingerprint plot of Boc-Ala(3-Cl)-OBn (**3**)

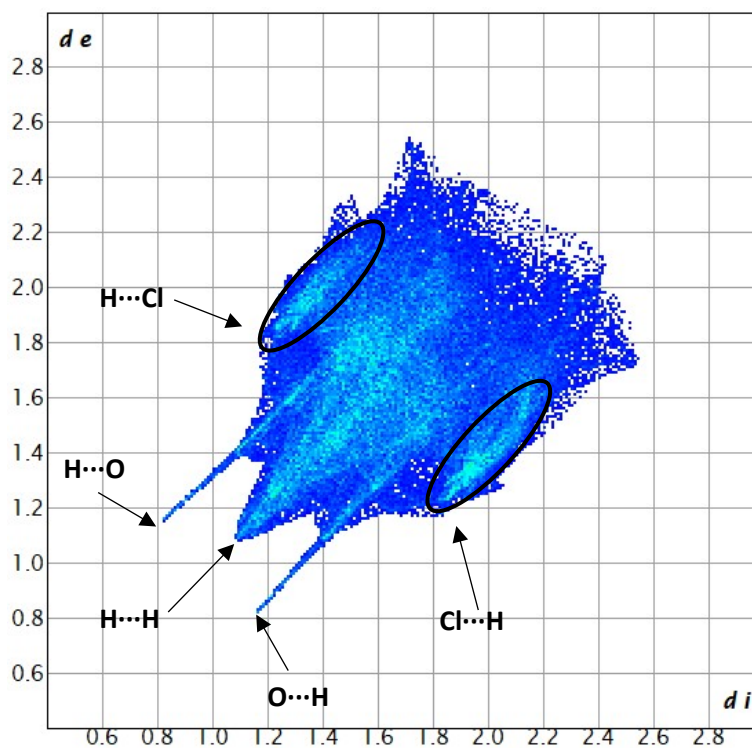


Figure S6. Fingerprint plot of **3**. Important intermolecular contacts are indicated with arrows.

Hirshfeld surface of Fmoc-Ala(3-Cl)-O^tBu (**4**)

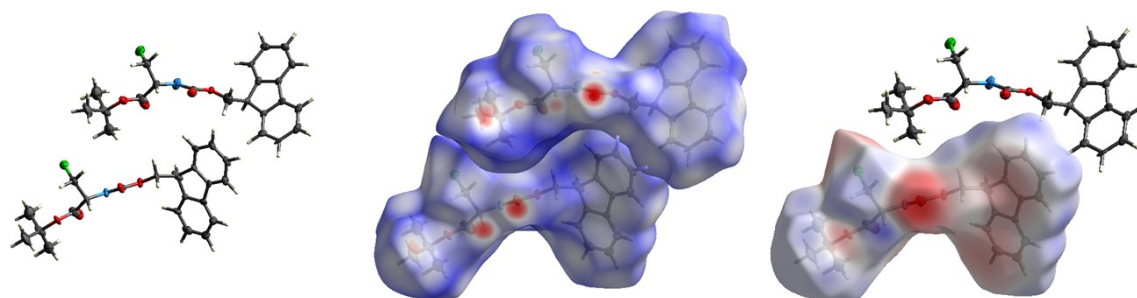


Figure S7. Molecular structures of **4** (left) and its Hirshfeld surface mapped with d_{norm} (middle) and ESP (right).

Fingerprint plot of Fmoc-Ala(3-Cl)-O^tBu (**4**)

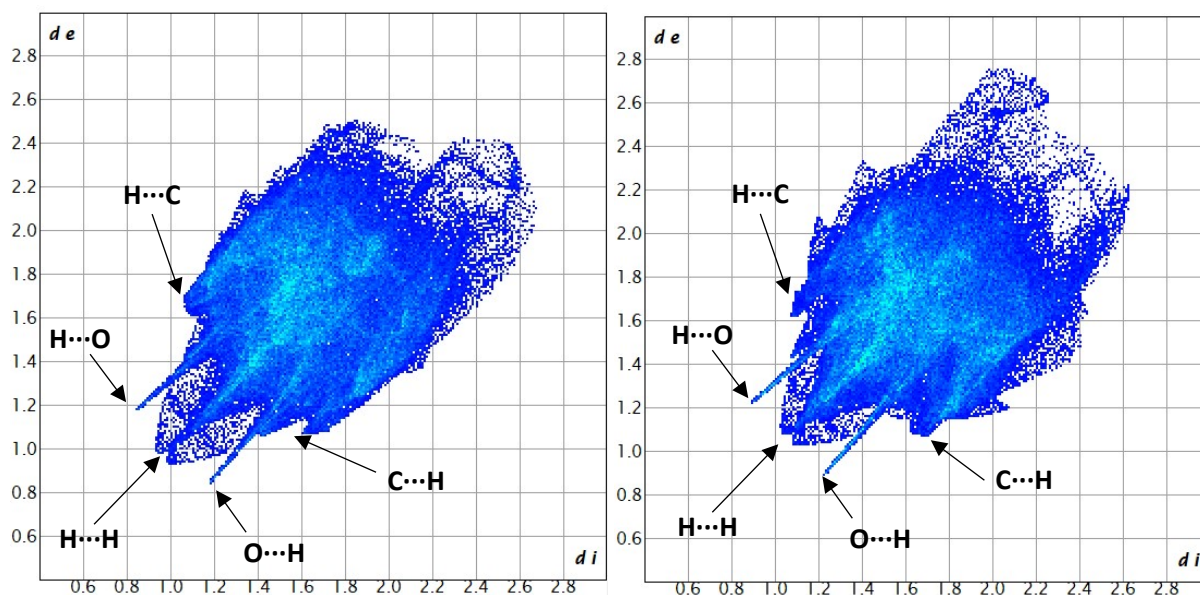


Figure S8. Fingerprint plots of two asymmetric molecules of **4**. The left plot corresponds to the top molecule and the right plot to the bottom molecule shown in Figure S7. Important intermolecular contacts are indicated with arrows.

Hirshfeld surface of Boc-Ala(3-I)-OMe (**5**)

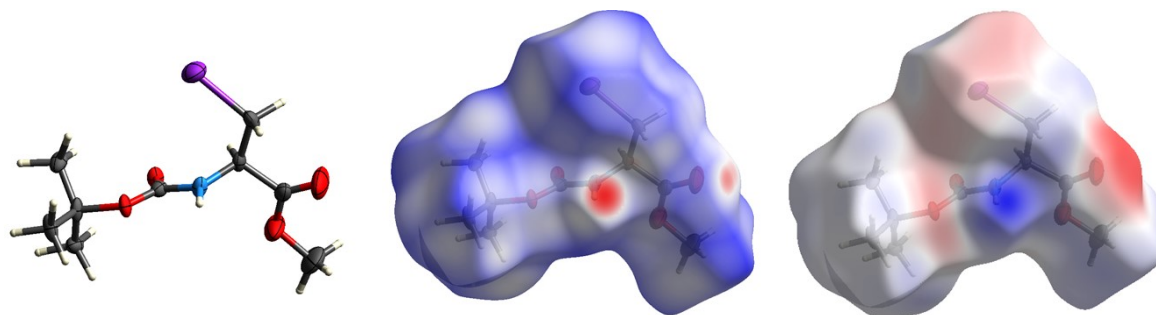


Figure S9. Molecular structure of **5** (left) and its Hirshfeld surface mapped with d_{norm} (middle) and ESP (right).

Fingerprint plot of Boc-Ala(3-I)-OMe (**5**)

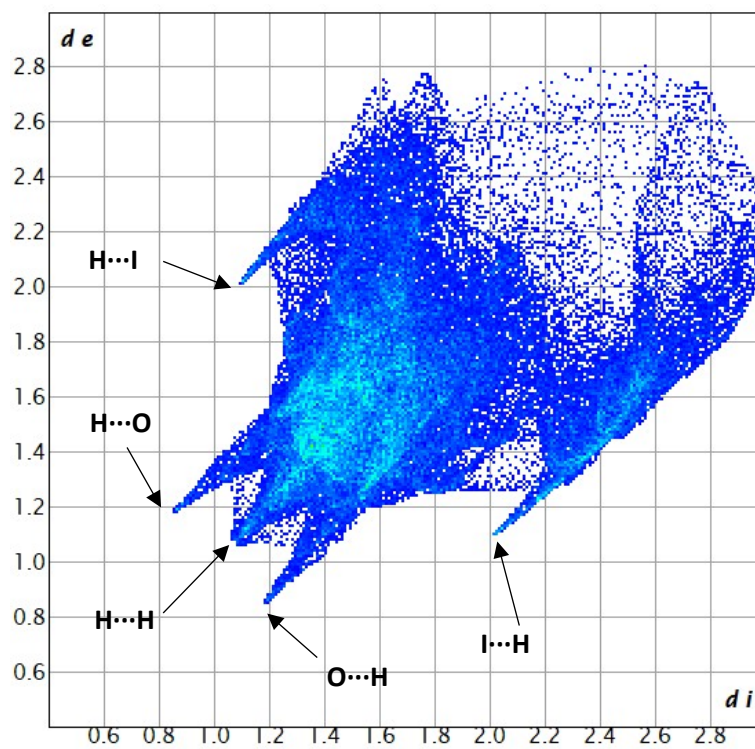


Figure S10. Fingerprint plot of **5**. Important intermolecular contacts are indicated with arrows.

Hirshfeld surface of Boc-Ala(3-I)-O^tBu (6)

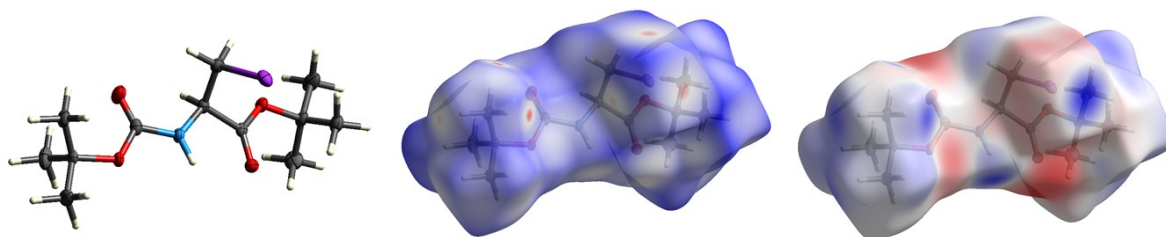


Figure S11. Molecular structure of **6** (left) and its Hirshfeld surface mapped with d_{norm} (middle) and ESP (right).

Fingerprint plot of Boc-Ala(3-I)-O^tBu (6)

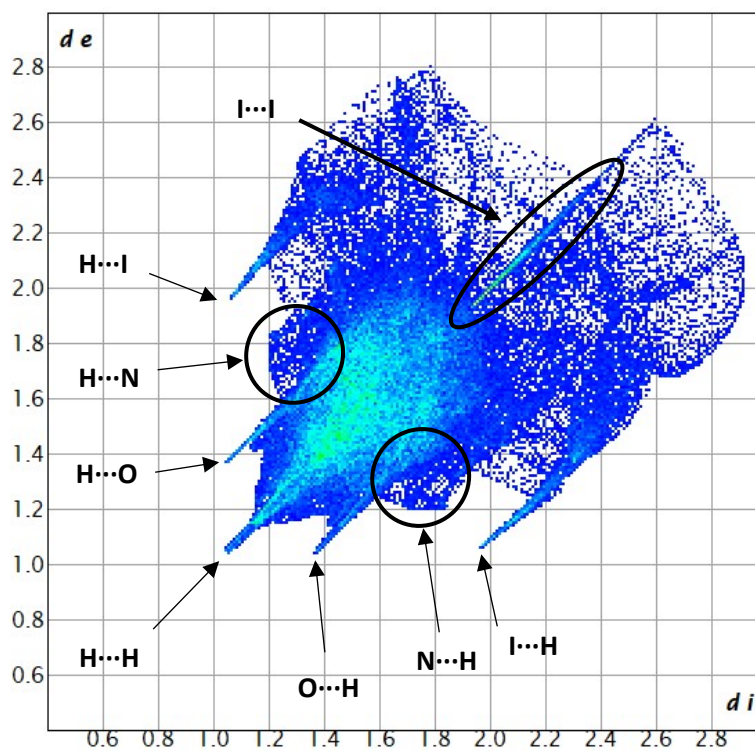


Figure S12. Fingerprint plot of **6**. Important intermolecular contacts are indicated with arrows.

Hirshfeld surface of Boc-Ala(3-I)-OBn (7)

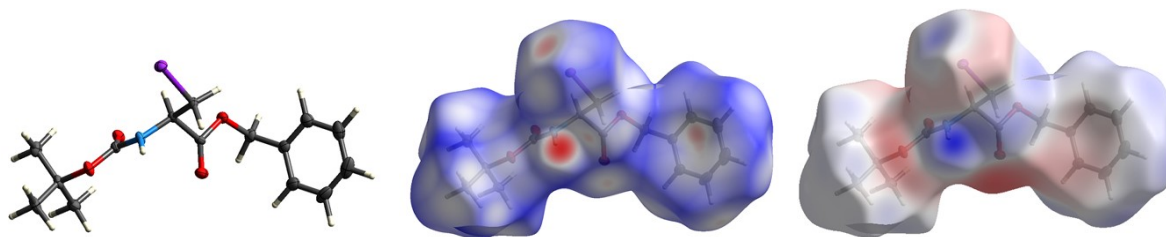


Figure S13. Molecular structure of **7** (left) and its Hirshfeld surface mapped with d_{norm} (middle) and ESP (right)

Fingerprint plot of Boc-Ala(3-I)-OBn (7)

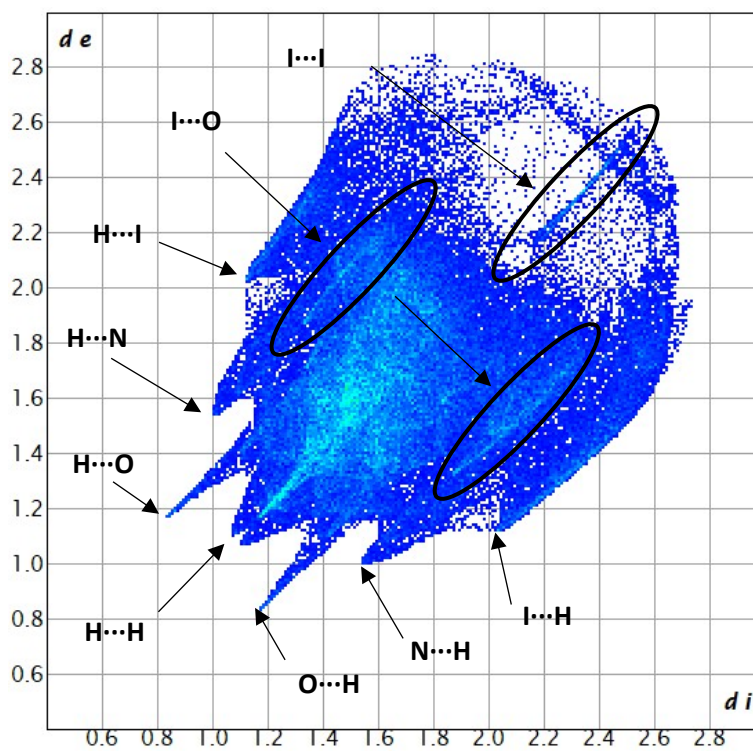


Figure S14. Fingerprint plot of **7**. Important intermolecular contacts are indicated with arrows.

Hirshfeld surface of Fmoc-Ala(3-I)-O^tBu (**8**)

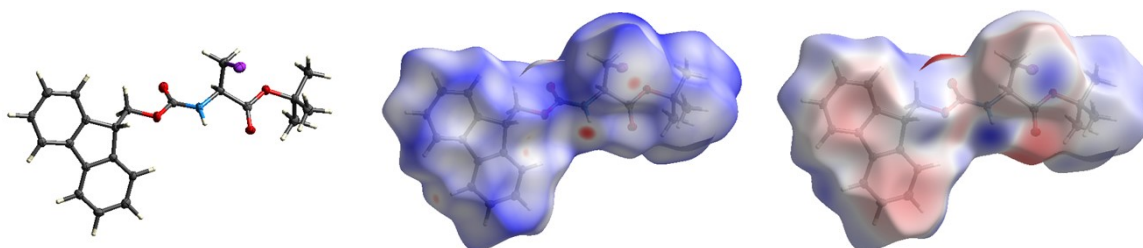


Figure S15. Molecular structure of **8** (left) and its Hirshfeld surface mapped with d_{norm} (middle) and ESP (right).

Fingerprint plot of Fmoc-Ala(3-I)-O^tBu (**8**)

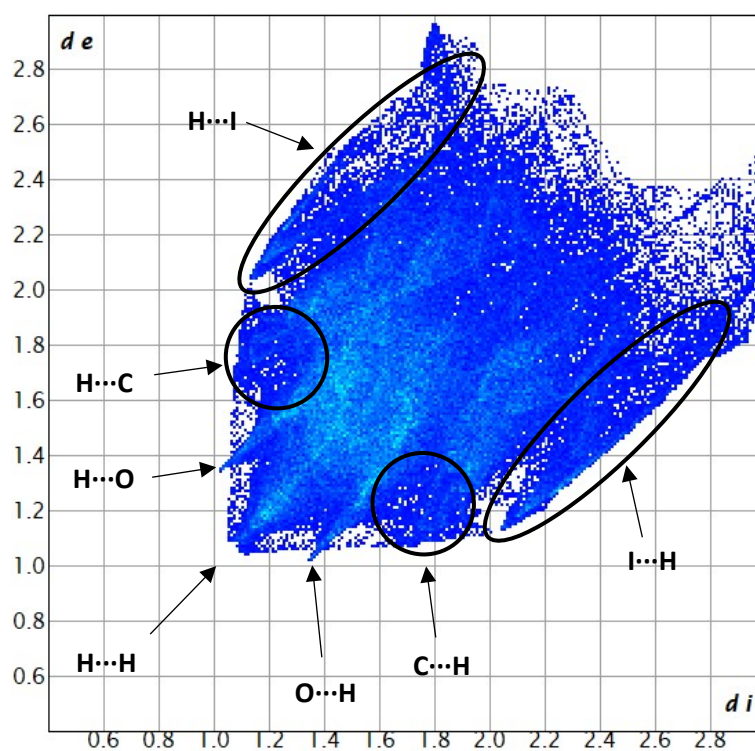


Figure S16. Fingerprint plot of **8**. Important intermolecular contacts are indicated with arrows.

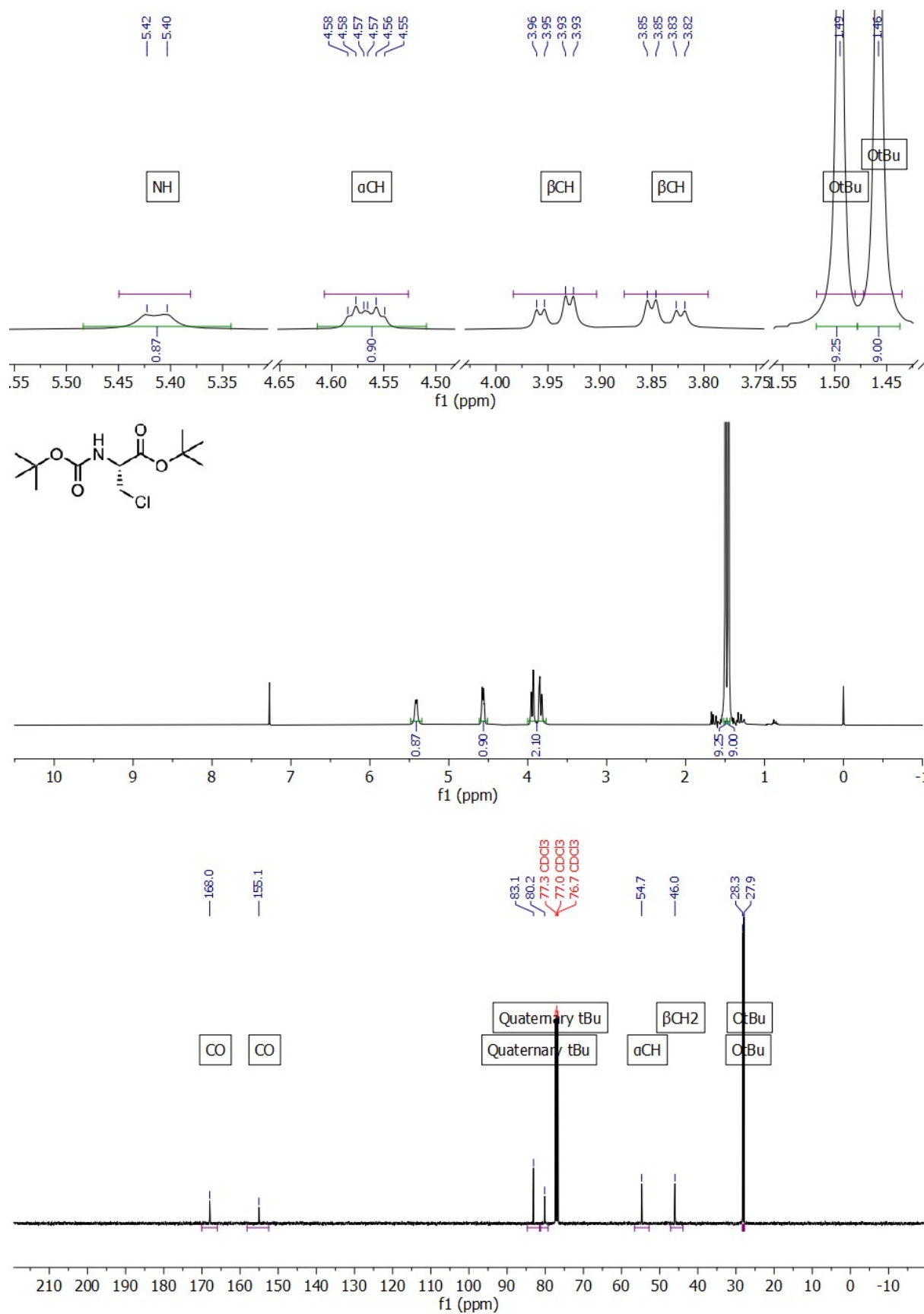


Figure S17. ¹H and ¹³C NMR spectra of Boc-Ala(3-Cl)-OtBu (2) (CDCl₃, 400/100 MHz, respectively).

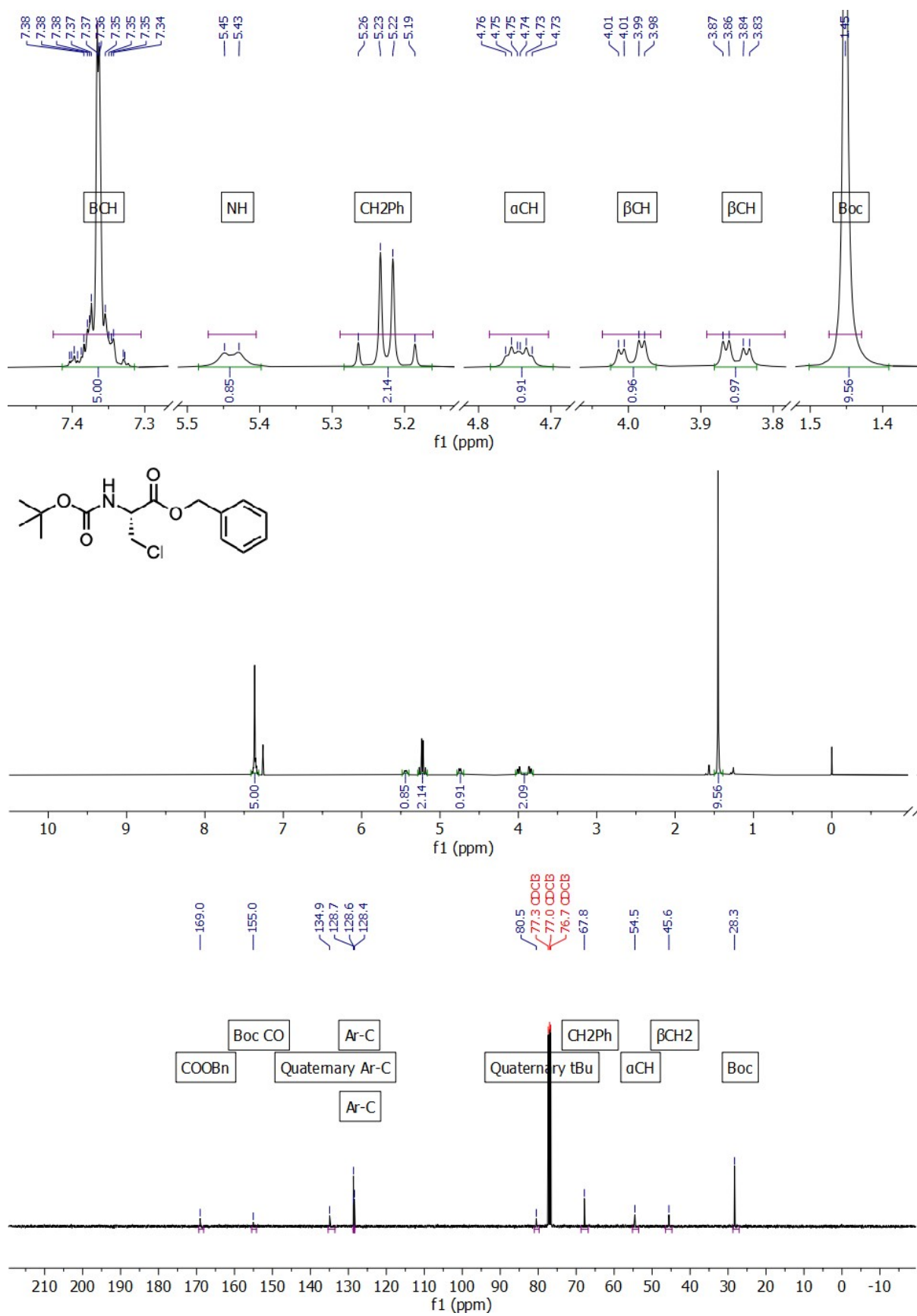


Figure S18. ¹H and ¹³C NMR spectra of Boc-Ala(3-Cl)-OBn (**3**) (CDCl₃, 400/100 MHz, respectively).