Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Isolation of hydrazine oxidation products via halogen bonding: C–I bond scission and crystal polymorphism

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Table SI1: Selected halogen bonding parameters (Å, °)

Y–X⋯A	*Y–X*	X⋯A	*Y–X⋯A*
		3	
C1–I1⋯N1	2.0995(3)	2.9640(3)	175.27(11)
C3–I2⋯N2	2.0902(3)	2.9732(3)	175.39(10)
		4	
C1–I1⋯N2	2.0911(4)	2.8937(4)	171.66(14)
C5–I2⋯N1	2.1016(4)	2.8930(4)	175.42(15)
		5	
C1–I1⋯I8	2.0831(13)	3.5736(11)	170.45(3)
C4–I2⋯I8	2.0743(11)	3.5514(11)	176.84(3)
C7–I3⋯I7	2.0673(11)	3.6138(12)	164.11(3)
C7–I3⋯I6	2.0673(11)	4.0232(11)	117.81(3)
C10–I4⋯I8	2.0894(11)	3.5364(10)	169.75(3)
C13–I5⋯I7	2.0661(16)	3.4506(13)	172.55(4)
C16–I6⋯I7	2.0629(14)	3.4109(13)	176.90(3)
C16–I6⋯I3	2.0629(14)	4.0232(11)	121.67(4)
		6	
C1–I1⋯I5	2.0992(3)	3.5655(3)	174.11(10)
C7–I3⋯I5	2.0925(3)	3.5691(3)	167.91(10)
C9–I4⋯I5	2.0960(3)	3.5961(3)	177.05(10)
		7	
C5–I2⋯I1	2.1014(5)	3.5186(4)	176.55(14)
C7–I3⋯I1	2.0937(5)	3.6262(5)	172.77(13)
		8	
C5–I2⋯I1	2.1081(2)	3.5156(2)	176.79(10)
C7–I3⋯I1	2.0972(2)	3.5664(2)	171.01(10)
C11–I4⋯I1	2.1017(2)	3.5148(2)	174.55(10)
C13–I5⋯I1	2.0918(2)	3.6731(2)	171.99(10)
		9	
C3–I18⋯I20	2.0987(2)	3.5575(5)	168.57(7)
C4–I19⋯I20	2.0964(2)	3.5589(5)	166.99(6)
		10	
C3–I2⋯I1	2.1053(5)	3.5317(10)	171.07(14)
C4–I3⋯I1	2.0949(5)	3.7556(10)	162.55(10)
		11	
C2–I1⋯I4	2.0850(3)	3.7492(3)	153.69(10)
C4–I2⋯I4	2.0967(3)	3.4409(3)	176.13(10)
C6–I3⋯I4	2.0883(3)	3.5445(3)	166.46(10)
		12	
C4–I2⋯I1	2.1066(4)	3.3932(4)	177.74(12)
C6–I3⋯I1	2.0907(4)	3.5683(4)	167.51(12)
C8–I4⋯I1	2.0821(4)	3.7193(4)	156.61(12)

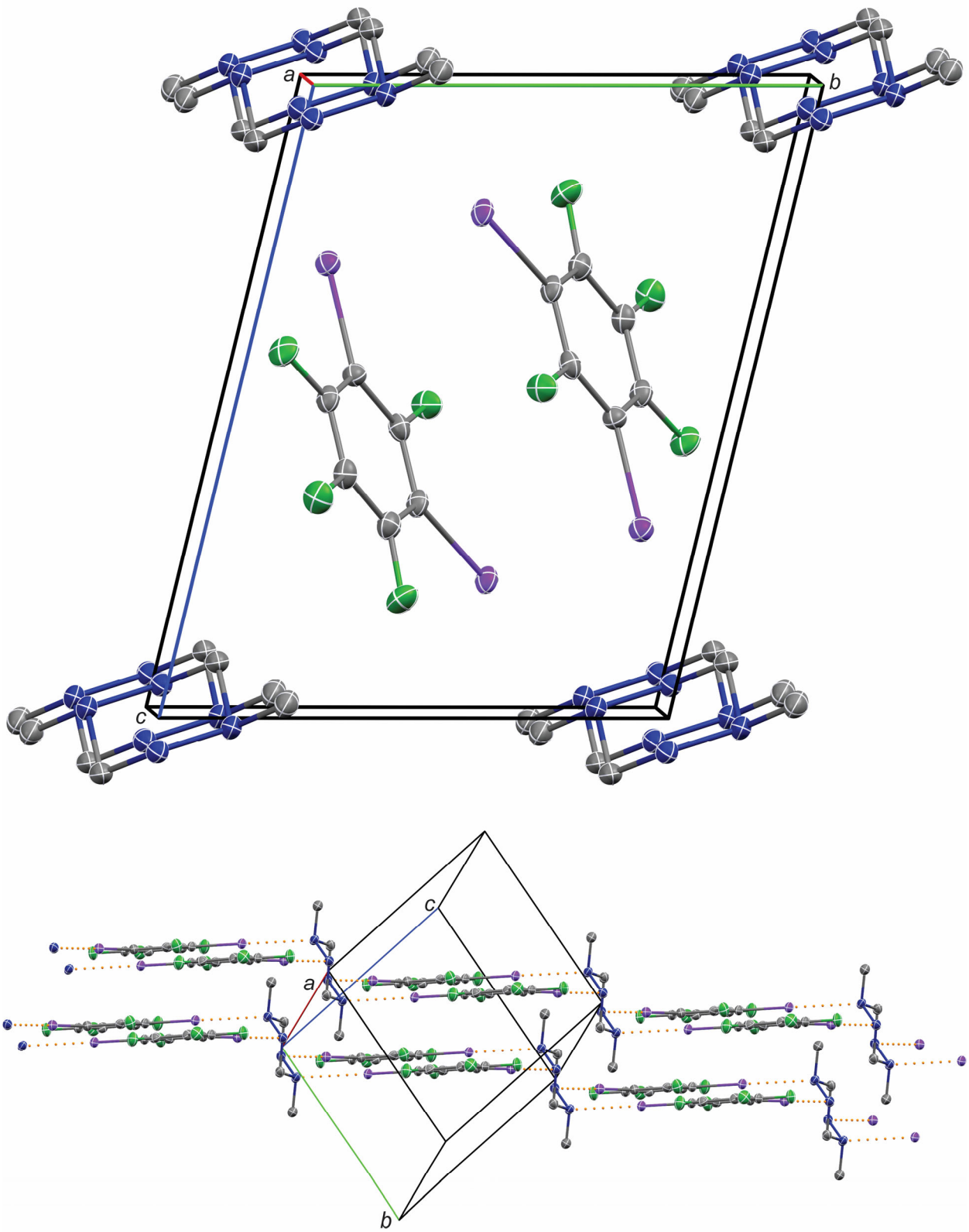

Figure SI1: Unit cell packing of 2(***m*-F$_4$DIB**)·(**HHDMTZ**) (**3**) as viewed down the *a* axis (top) and halogen bonding chains (bottom). Hydrogen atoms have been omitted for clarity. Thermal ellipsoids are shown at the 50% probability level.

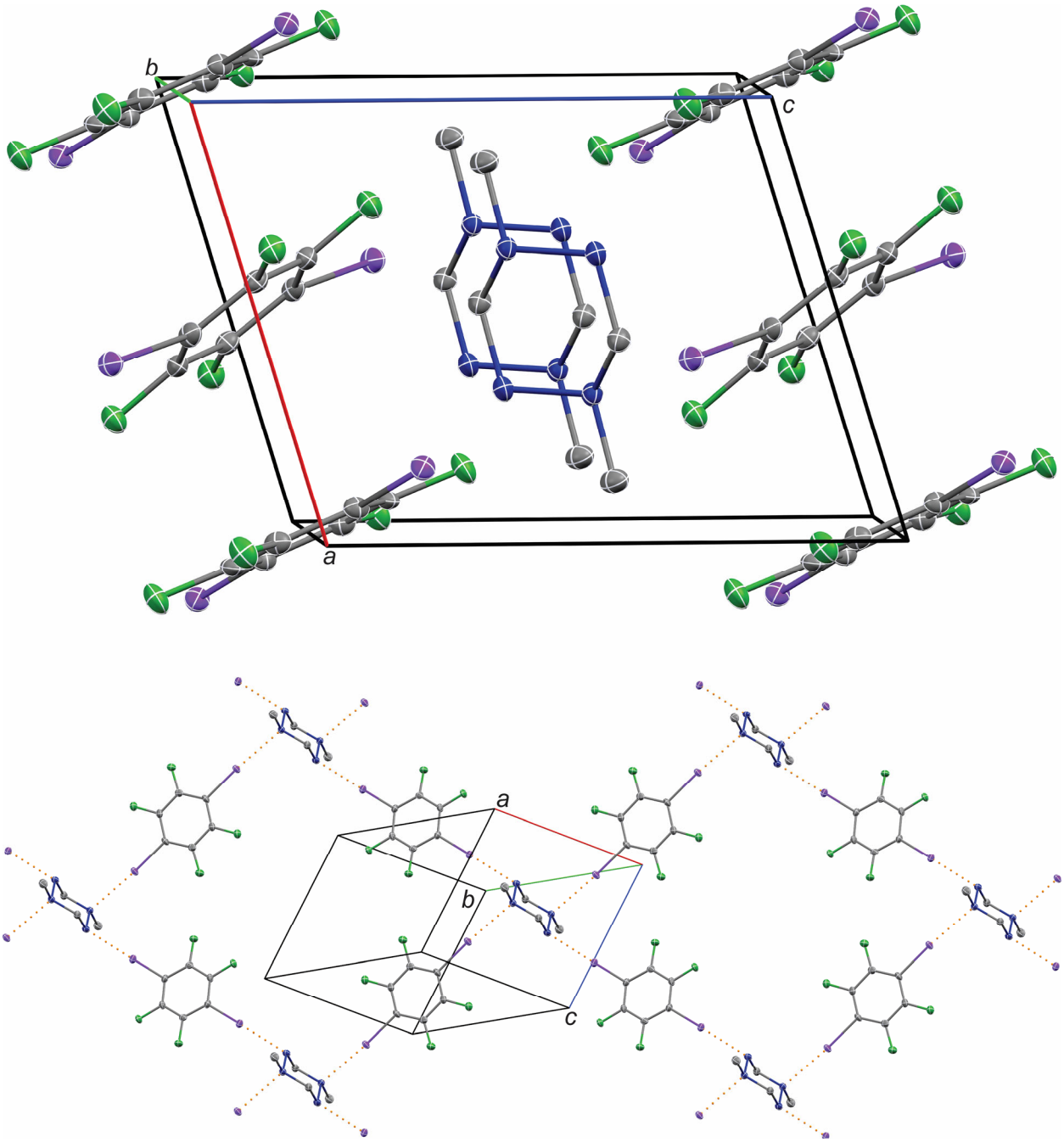

Figure SI2: Unit cell packing of 2(***p*-F$_4$DIB**)·(**HHDMTZ**) (**4**) as viewed down the *b* axis (top) and halogen bonding sheets (bottom). Hydrogen atoms have been omitted for clarity. Thermal ellipsoids are shown at the 50% probability level.

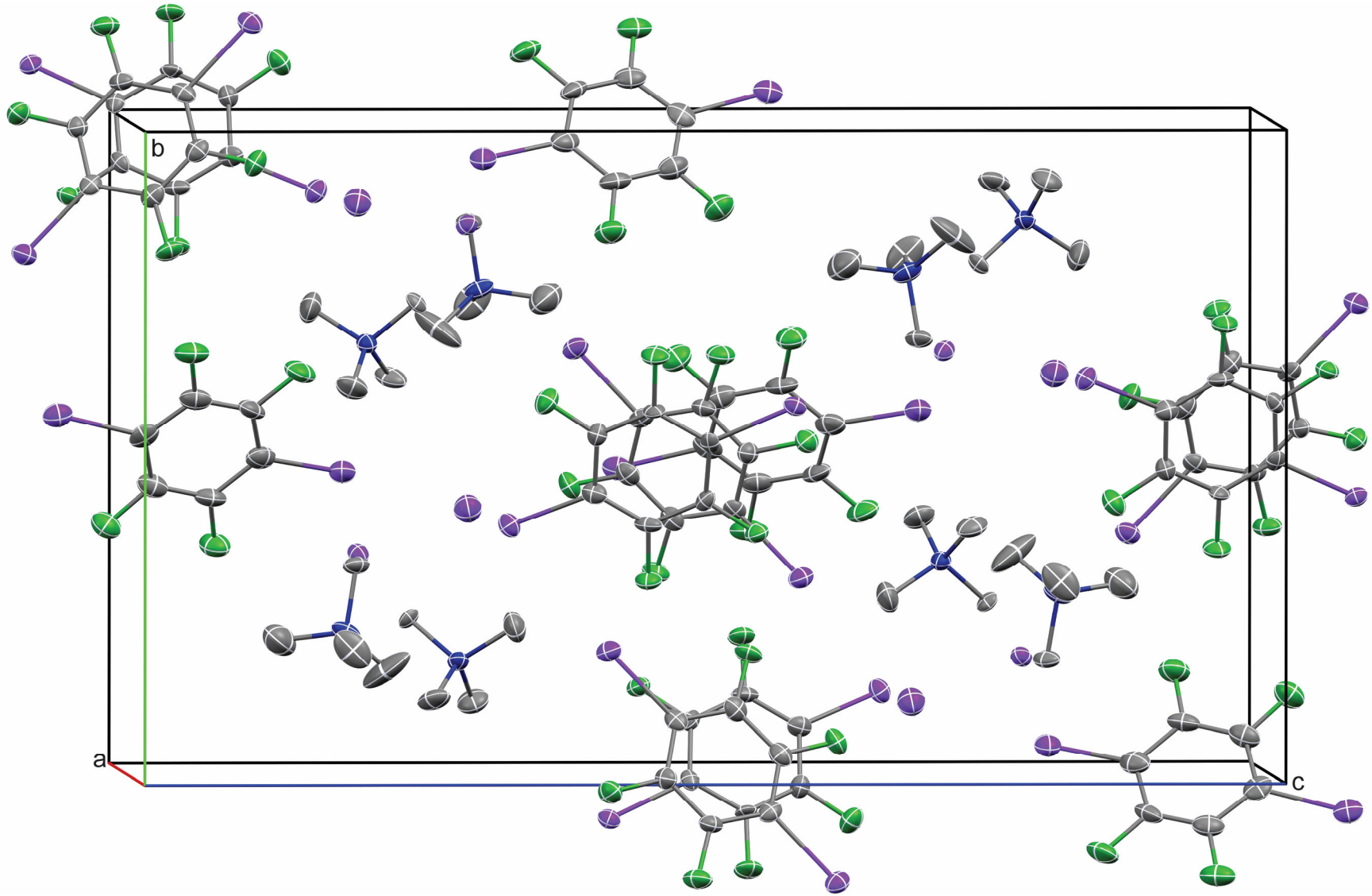

Figure SI3: Unit cell packing of 3(***p*-F$_4$DIB**)·(**NMe$_4$I**) (**5**) as viewed down the ***a*** axis. Hydrogen atoms have been omitted for clarity. Thermal ellipsoids are shown at the 50% probability level.

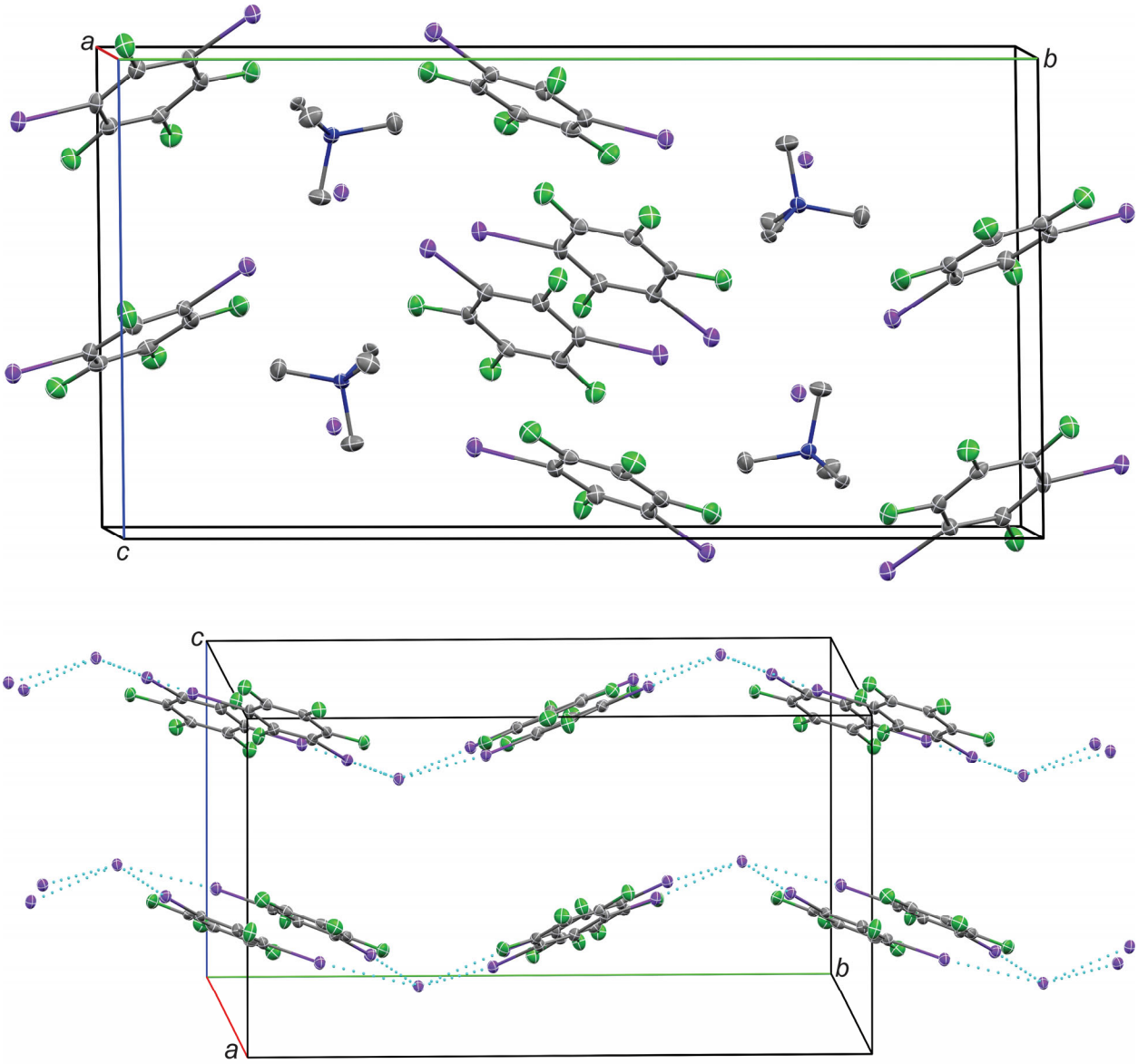

Figure SI4: Unit cell packing of 2(***m*-F$_4$DIB**)·(**NMe$_4$I**) (**6**) as viewed down the ***a*** axis (top) and halogen bonding ribbons (bottom). Hydrogen atoms have been omitted for clarity. Thermal ellipsoids are shown at the 50% probability level.

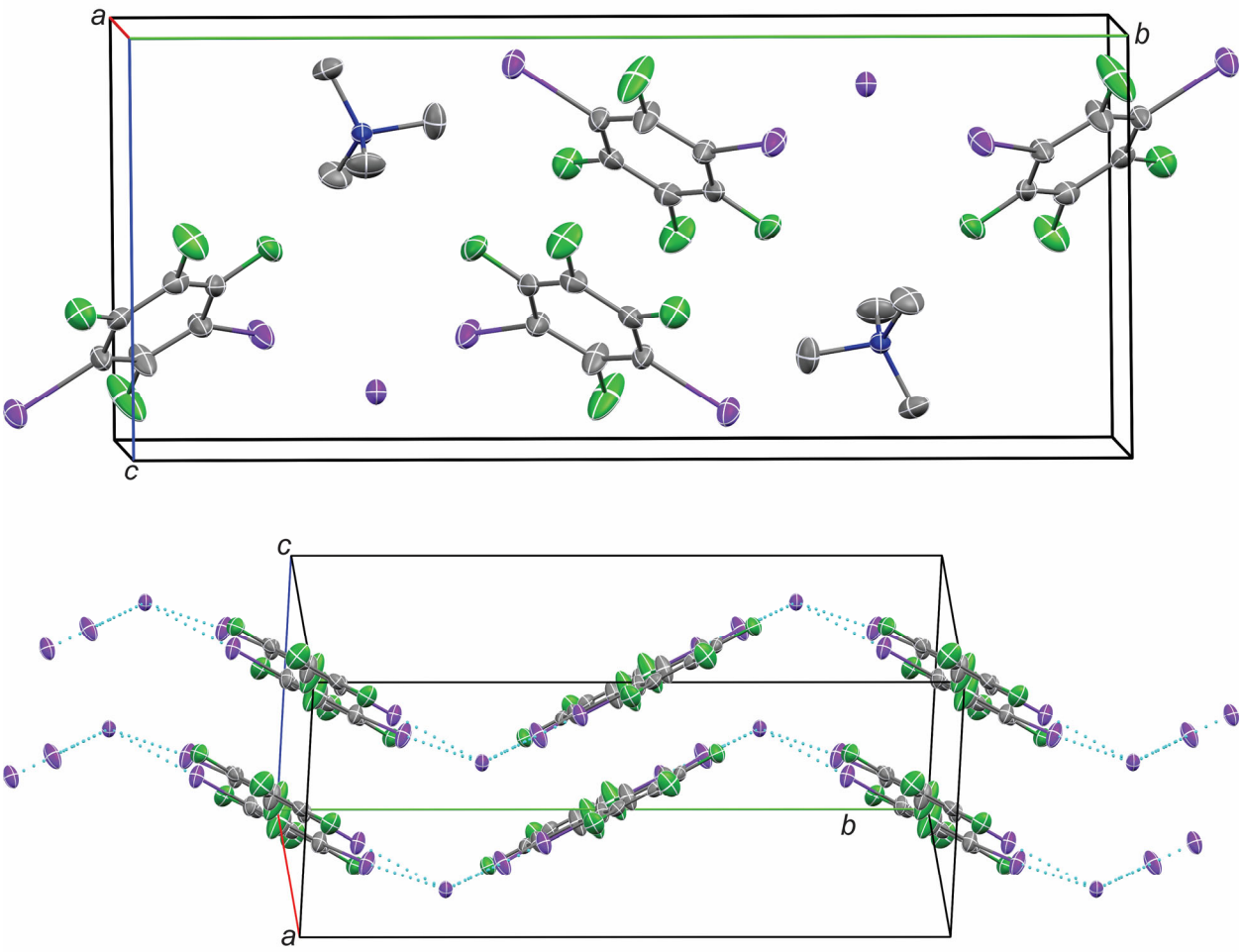

Figure SI5: Unit cell packing of 2(***m*-F$_4$DIB**)·(**NMe$_4$I**) (**7**) as viewed down the *a* axis (top) and halogen bonding ribbons (bottom). Hydrogen atoms have been omitted for clarity. Thermal ellipsoids are shown at the 50% probability level.

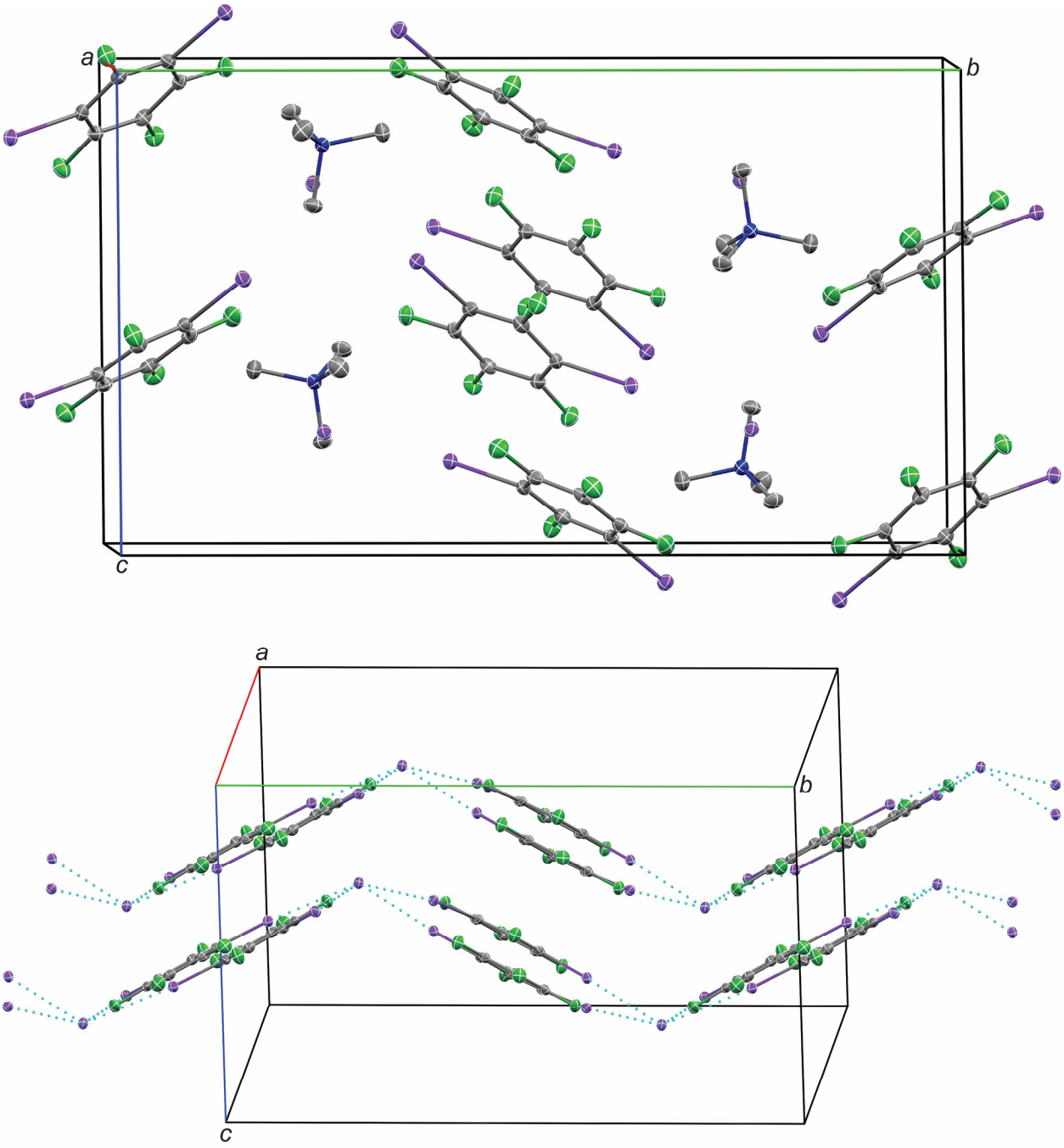

Figure SI6: Unit cell packing of 2(***m*-F$_4$DIB**)·(**NMe$_4$I**) (**8**) as viewed down the *a* axis (top) and halogen bonding ribbons (bottom). Hydrogen atoms have been omitted for clarity. Thermal ellipsoids are shown at the 50% probability level.

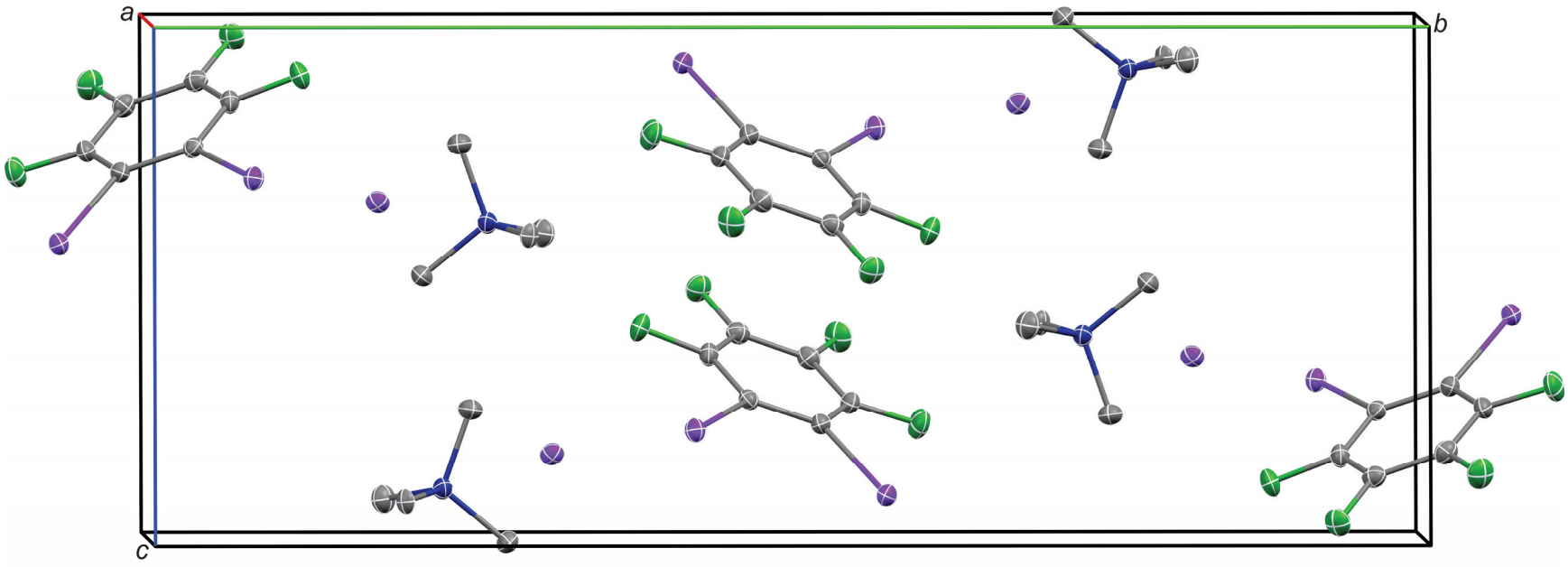

Figure SI7: Unit cell packing of (***o*-F$_4$DIB**)·(**NMe$_4$I**) (**9**) as viewed down the *a* axis. Hydrogen atoms have been omitted for clarity. Thermal ellipsoids are shown at the 50% probability level.

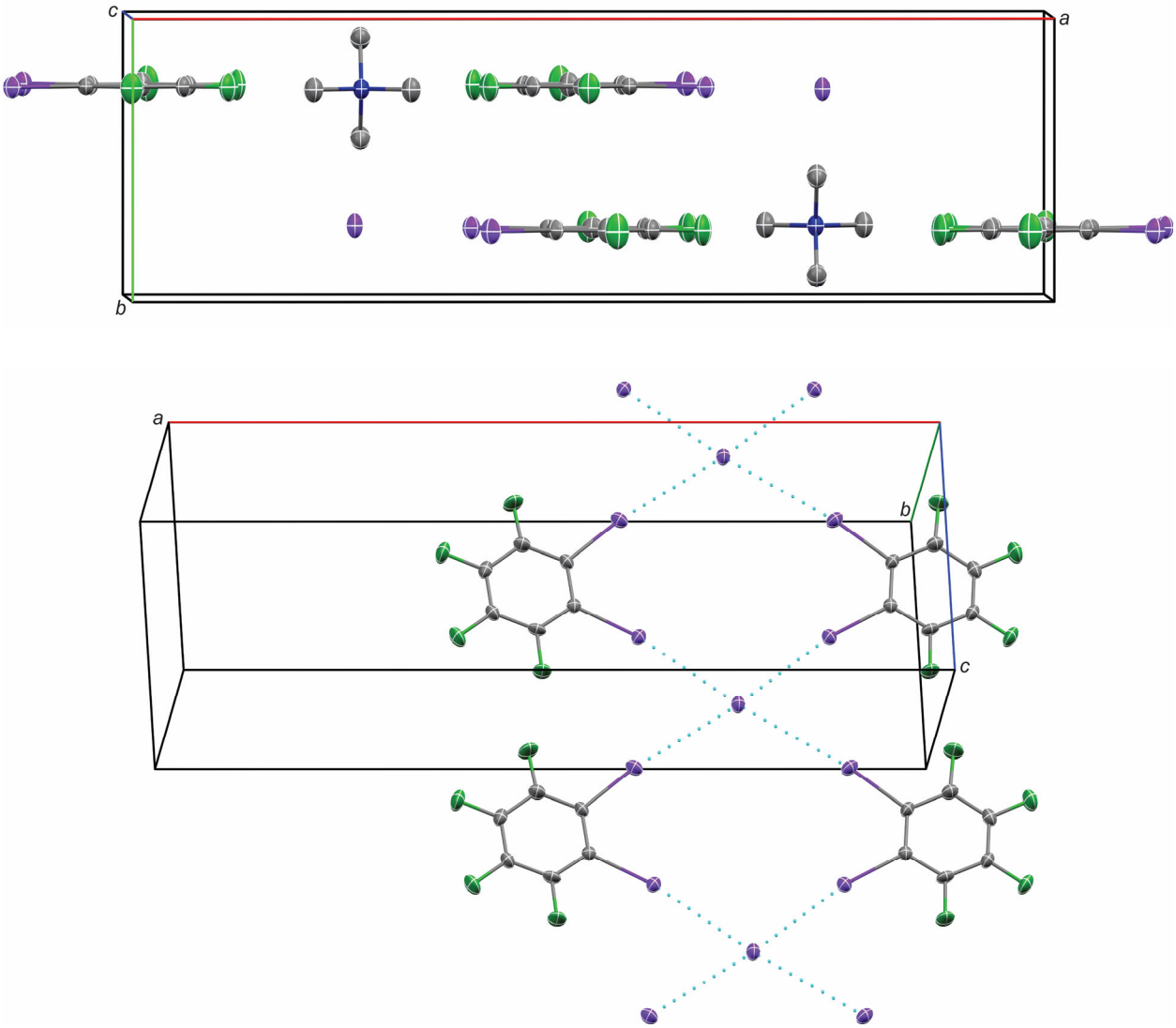

Figure SI8: Unit cell packing of 2(***o*-F$_4$DIB**)·(**NMe$_4$I**) (**10**) as viewed down the *c* axis (top) halogen bonding ribbons (bottom). Hydrogen atoms have been omitted for clarity. Thermal ellipsoids are shown at the 50% probability level.

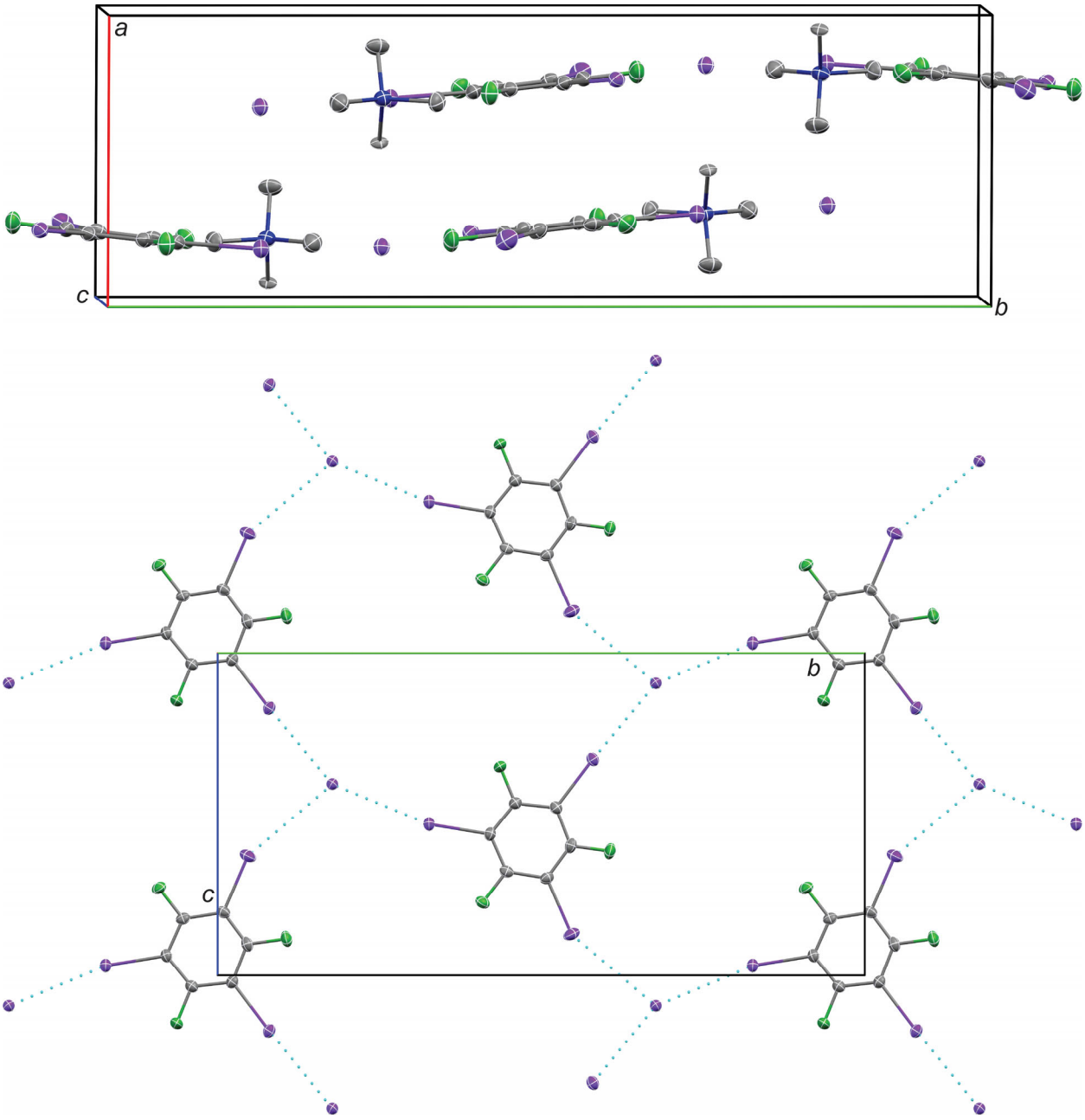

Figure SI9: Unit cell packing of (**135-F_3I_3B**)·(**NMe_4I**) (**11**) as viewed down the *c* axis (top) and halogen bonding sheets as viewed down the *a* axis (bottom). Hydrogen atoms have been omitted for clarity. Thermal ellipsoids are shown at the 50% probability level.

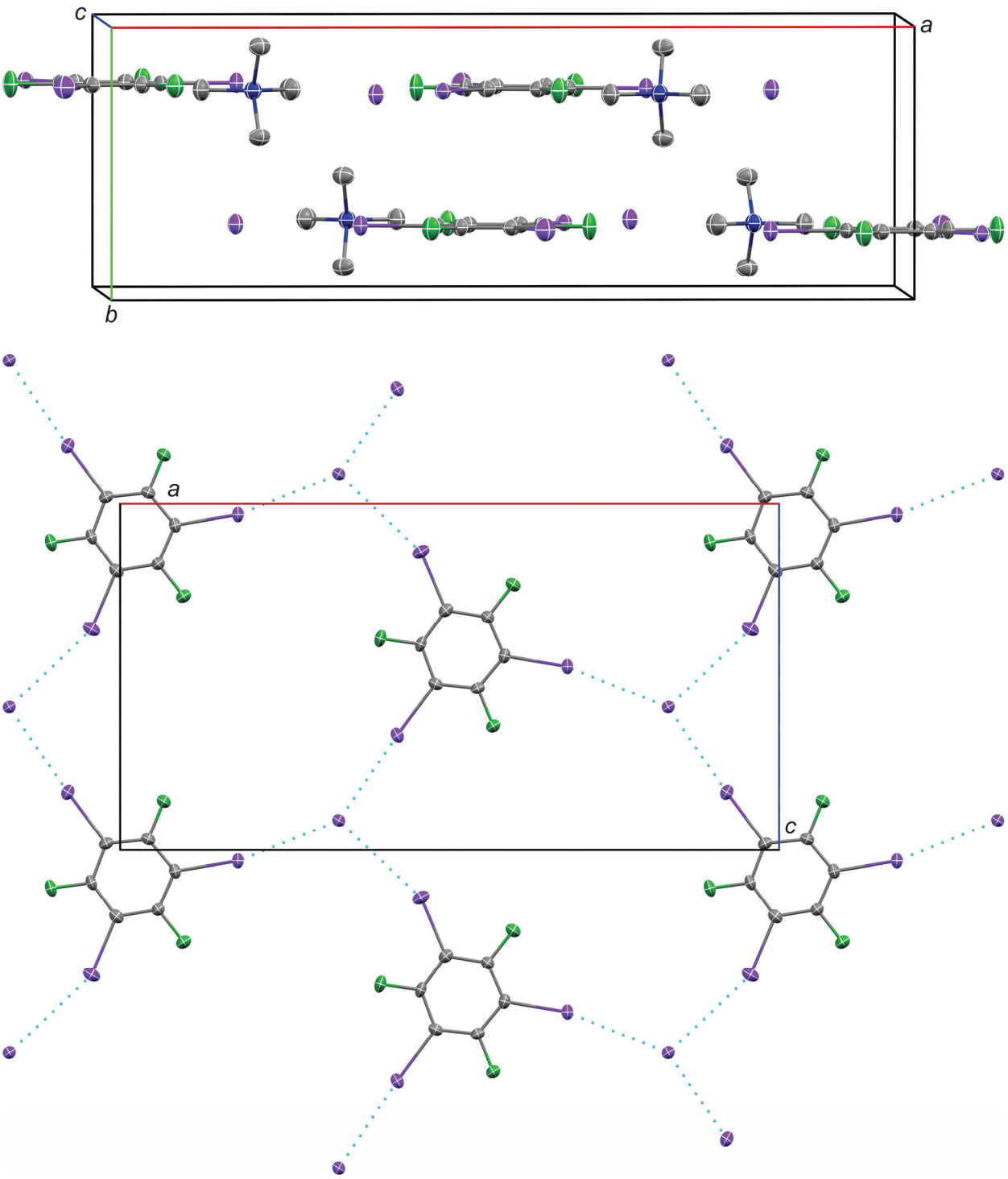

Figure SI10: Unit cell packing of (**135-F_3I_3B**)·(**NMe_4I**) (**12**) as viewed down the *c* axis (top) and . halogen bonding sheets as viewed down the *b* axis (bottom). Hydrogen atoms have been omitted for clarity. Thermal ellipsoids are shown at the 50% probability level.