

# **X-ray diffraction and QTAIM calculations of the non-covalent intermolecular fluorine-fluorine interactions in tris(trifluoroacetylacetonato)-manganese(III).**

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## **Supplementary information**

### **Table of Contents**

Table 1. Crystal data and structure refinement for mo_roxf02_0ma_a. ....	2
Table 2. Atomic coordinates .....	3
Table 3. Bond lengths [Å] and angles [°] for mo_roxf02_0ma_a. ....	5
Table 4. Anisotropic displacement parameters.....	11
Table 5. Hydrogen coordinates ( x 10 <sup>4</sup> ) and isotropic displacement parameters (Å <sup>2</sup> x 10 <sup>3</sup> ) for mo_roxf02_0ma_a.....	13
Table 6. Torsion angles [°] for mo_roxf02_0ma_a. ....	14
Table 7. Hydrogen bonds for mo_roxf02_0ma_a [Å and °].....	17

**Table 1. Crystal data and structure refinement for mo\_roxf02\_0ma\_a.**

Identification code	shelx	
Empirical formula	C <sub>15</sub> H <sub>12</sub> F <sub>9</sub> Mn O <sub>6</sub>	
Formula weight	514.19	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P c a 2 <sub>1</sub>	
Unit cell dimensions	a = 14.6540(10) Å	α = 90°.
	b = 19.8572(8) Å	β = 90°.
	c = 13.3915(7) Å	γ = 90°.
Volume	3896.8(4) Å <sup>3</sup>	
Z	8	
Density (calculated)	1.753 Mg/m <sup>3</sup>	
Absorption coefficient	0.792 mm <sup>-1</sup>	
F(000)	2048	
Crystal size	0.400 x 0.200 x 0.200 mm <sup>3</sup>	
Theta range for data collection	2.301 to 25.113°.	
Index ranges	-17<=h<=17, -23<=k<=23, -15<=l<=15	
Reflections collected	128022	
Independent reflections	6943 [R(int) = 0.0487]	
Completeness to theta = 25.113°	99.9 %	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	6943 / 1 / 566	
Goodness-of-fit on F <sup>2</sup>	1.071	
Final R indices [I>2sigma(I)]	R1 = 0.0543, wR2 = 0.1505	
R indices (all data)	R1 = 0.0563, wR2 = 0.1527	
Absolute structure parameter	0.10(3)	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.428 and -0.531 e.Å <sup>-3</sup>	

## Table 2. Atomic coordinates

Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for mo\_roxf02\_0ma\_a.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	U(eq)
Mn(1)	3721(1)	4810(1)	14957(1)	23(1)
Mn'1	6209(1)	10205(1)	12546(1)	25(1)
O(1)	3067(3)	5529(2)	15725(3)	34(1)
O(2)	2688(3)	4761(2)	14012(3)	31(1)
O(3)	4268(3)	5526(2)	14123(3)	34(1)
O(4)	4761(3)	4875(2)	15879(3)	30(1)
O(5)	4354(3)	4077(2)	14195(3)	32(1)
O(6)	3155(3)	4104(2)	15828(3)	35(1)
O'1	6777(3)	9501(2)	13314(3)	34(1)
O'2	7277(3)	10197(2)	11603(3)	34(1)
O'3	5567(3)	9463(3)	11750(3)	40(1)
O'4	5161(3)	10224(2)	13486(4)	35(1)
O'5	5641(3)	10900(2)	11741(3)	32(1)
O'6	6845(3)	10939(2)	13381(3)	36(1)
F(1)	2113(4)	6258(3)	17041(3)	70(2)
F(2)	1234(4)	6634(3)	15914(5)	80(2)
F(3)	2616(5)	6928(2)	15933(5)	89(2)
F(4)	4211(4)	6912(2)	13749(4)	69(2)
F(5)	5118(4)	6353(2)	12808(3)	58(1)
F(6)	5637(4)	6950(3)	14016(4)	75(2)
F(7)	4859(5)	2385(3)	13885(6)	93(2)
F(8)	4347(4)	3019(3)	12752(4)	84(2)
F(9)	5597(4)	3247(3)	13454(6)	94(2)
F'1	6668(4)	8169(3)	13715(6)	87(2)
F'2	7724(4)	8627(2)	14547(3)	66(2)
F'3	8009(5)	8018(3)	13258(4)	89(2)
F'4	3922(7)	8220(4)	11710(7)	139(4)
F'5	4723(6)	8595(4)	10544(5)	98(2)
F'6	5307(9)	8029(4)	11676(8)	181(6)

F'7	5527(4)	12570(2)	10940(5)	73(2)
F'8	4430(3)	11880(3)	11111(4)	65(1)
F'9	5487(4)	11683(3)	10070(4)	79(2)
C(1)	2346(4)	5812(3)	15423(5)	30(1)
C(2)	1812(4)	5667(3)	14630(5)	33(1)
C(3)	2018(4)	5145(3)	13948(5)	27(1)
C(4)	4875(4)	5941(3)	14435(5)	30(1)
C(5)	5399(4)	5888(3)	15273(5)	33(1)
C(6)	5342(4)	5349(3)	15949(5)	27(1)
C(7)	4277(4)	3448(3)	14348(5)	29(1)
C(8)	3780(4)	3130(3)	15101(6)	39(2)
C(9)	3247(4)	3466(3)	15796(5)	33(1)
C(10)	2074(6)	6410(4)	16090(6)	47(2)
C(11)	4979(6)	6542(3)	13752(6)	42(2)
C(12)	4802(4)	3018(3)	13616(6)	39(2)
C(13)	1400(5)	5044(4)	13067(5)	37(2)
C(14)	5999(5)	5307(3)	16809(5)	36(2)
C(15)	2740(5)	3068(4)	16550(6)	48(2)
C'1	7382(4)	9105(3)	12969(5)	31(1)
C'2	7925(5)	9175(3)	12159(5)	39(2)
C'3	7868(4)	9756(3)	11521(5)	31(1)
C'4	4911(5)	9115(3)	12104(5)	34(1)
C'5	4392(5)	9243(3)	12939(5)	37(2)
C'6	4530(4)	9790(3)	13581(5)	28(1)
C'7	5842(4)	11526(3)	11764(5)	32(1)
C'8	6408(5)	11867(3)	12397(6)	41(2)
C'9	6856(4)	11565(3)	13205(5)	36(2)
C'10	7463(6)	8468(3)	13631(6)	49(2)
C'11	4702(8)	8482(4)	11503(7)	65(3)
C'12	5323(5)	11914(3)	10947(6)	40(2)
C'13	8556(5)	9837(4)	10708(5)	44(2)
C'14	3891(5)	9887(4)	14460(6)	39(2)
C'15	7381(6)	11995(4)	13933(7)	51(2)

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**Table 3. Bond lengths [Å] and angles [°] for mo\_roxf02\_0ma\_a.**

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Mn(1)-O(4)	1.966(5)
Mn(1)-O(2)	1.975(5)
Mn(1)-O(3)	1.978(5)
Mn(1)-O(1)	2.004(5)
Mn(1)-O(6)	2.004(5)
Mn(1)-O(5)	2.006(4)
Mn'1-O'1	1.924(4)
Mn'1-O'5	1.939(4)
Mn'1-O'4	1.985(5)
Mn'1-O'2	2.012(5)
Mn'1-O'3	2.047(5)
Mn'1-O'6	2.061(5)
O(1)-C(1)	1.264(8)
O(2)-C(3)	1.246(7)
O(3)-C(4)	1.282(8)
O(4)-C(6)	1.272(7)
O(5)-C(7)	1.269(7)
O(6)-C(9)	1.276(8)
O'1-C'1	1.272(8)
O'2-C'3	1.237(7)
O'3-C'4	1.275(9)
O'4-C'6	1.271(7)
O'5-C'7	1.279(8)
O'6-C'9	1.264(8)
F(1)-C(10)	1.310(9)
F(2)-C(10)	1.330(9)
F(3)-C(10)	1.317(10)
F(4)-C(11)	1.345(9)
F(5)-C(11)	1.334(9)
F(6)-C(11)	1.310(9)
F(7)-C(12)	1.309(9)

F(8)-C(12)	1.337(10)
F(9)-C(12)	1.270(9)
F'1-C'10	1.313(10)
F'2-C'10	1.324(9)
F'3-C'10	1.299(9)
F'4-C'11	1.287(12)
F'5-C'11	1.305(11)
F'6-C'11	1.284(12)
F'7-C'12	1.338(8)
F'8-C'12	1.330(9)
F'9-C'12	1.283(9)
C(1)-C(2)	1.349(9)
C(1)-C(10)	1.538(9)
C(2)-C(3)	1.415(9)
C(3)-C(13)	1.501(9)
C(4)-C(5)	1.365(9)
C(4)-C(11)	1.510(9)
C(5)-C(6)	1.404(9)
C(6)-C(14)	1.504(9)
C(7)-C(8)	1.395(10)
C(7)-C(12)	1.511(9)
C(8)-C(9)	1.386(10)
C(9)-C(15)	1.481(10)
C'1-C'2	1.353(10)
C'1-C'10	1.549(9)
C'2-C'3	1.438(9)
C'3-C'13	1.493(10)
C'4-C'5	1.375(9)
C'4-C'11	1.524(10)
C'5-C'6	1.401(9)
C'6-C'14	1.517(10)
C'7-C'8	1.366(10)
C'7-C'12	1.538(9)
C'8-C'9	1.401(11)
C'9-C'15	1.507(10)

O(4)-Mn(1)-O(2)	178.73(19)
O(4)-Mn(1)-O(3)	89.62(18)
O(2)-Mn(1)-O(3)	89.10(18)
O(4)-Mn(1)-O(1)	90.06(17)
O(2)-Mn(1)-O(1)	89.88(17)
O(3)-Mn(1)-O(1)	88.33(18)
O(4)-Mn(1)-O(6)	90.03(18)
O(2)-Mn(1)-O(6)	91.24(19)
O(3)-Mn(1)-O(6)	178.41(19)
O(1)-Mn(1)-O(6)	90.1(2)
O(4)-Mn(1)-O(5)	90.52(18)
O(2)-Mn(1)-O(5)	89.56(18)
O(3)-Mn(1)-O(5)	92.72(19)
O(1)-Mn(1)-O(5)	178.80(19)
O(6)-Mn(1)-O(5)	88.84(17)
O'1-Mn'1-O'5	178.48(19)
O'1-Mn'1-O'4	90.58(18)
O'5-Mn'1-O'4	90.4(2)
O'1-Mn'1-O'2	89.62(18)
O'5-Mn'1-O'2	89.44(19)
O'4-Mn'1-O'2	179.16(19)
O'1-Mn'1-O'3	87.40(19)
O'5-Mn'1-O'3	91.4(2)
O'4-Mn'1-O'3	89.38(19)
O'2-Mn'1-O'3	91.45(18)
O'1-Mn'1-O'6	91.7(2)
O'5-Mn'1-O'6	89.54(18)
O'4-Mn'1-O'6	89.55(18)
O'2-Mn'1-O'6	89.63(19)
O'3-Mn'1-O'6	178.6(2)
C(1)-O(1)-Mn(1)	123.5(4)
C(3)-O(2)-Mn(1)	128.1(4)
C(4)-O(3)-Mn(1)	124.0(4)
C(6)-O(4)-Mn(1)	127.8(4)
C(7)-O(5)-Mn(1)	126.2(4)
C(9)-O(6)-Mn(1)	129.2(5)

C'1-O'1-Mn'1	123.8(4)
C'3-O'2-Mn'1	127.3(4)
C'4-O'3-Mn'1	122.8(4)
C'6-O'4-Mn'1	127.8(4)
C'7-O'5-Mn'1	125.4(4)
C'9-O'6-Mn'1	126.9(4)
O(1)-C(1)-C(2)	129.9(6)
O(1)-C(1)-C(10)	112.0(6)
C(2)-C(1)-C(10)	118.1(6)
C(1)-C(2)-C(3)	122.7(6)
O(2)-C(3)-C(2)	124.9(6)
O(2)-C(3)-C(13)	116.6(6)
C(2)-C(3)-C(13)	118.5(6)
O(3)-C(4)-C(5)	127.5(6)
O(3)-C(4)-C(11)	112.3(6)
C(5)-C(4)-C(11)	120.2(6)
C(4)-C(5)-C(6)	123.8(6)
O(4)-C(6)-C(5)	123.8(6)
O(4)-C(6)-C(14)	116.4(6)
C(5)-C(6)-C(14)	119.8(6)
O(5)-C(7)-C(8)	127.5(6)
O(5)-C(7)-C(12)	113.9(6)
C(8)-C(7)-C(12)	118.6(6)
C(9)-C(8)-C(7)	124.2(6)
O(6)-C(9)-C(8)	124.0(6)
O(6)-C(9)-C(15)	117.0(6)
C(8)-C(9)-C(15)	119.0(6)
F(1)-C(10)-F(3)	108.0(7)
F(1)-C(10)-F(2)	106.8(7)
F(3)-C(10)-F(2)	105.6(7)
F(1)-C(10)-C(1)	112.1(6)
F(3)-C(10)-C(1)	110.7(7)
F(2)-C(10)-C(1)	113.2(6)
F(6)-C(11)-F(5)	108.5(7)
F(6)-C(11)-F(4)	106.1(6)
F(5)-C(11)-F(4)	106.2(6)

F(6)-C(11)-C(4)	113.6(6)
F(5)-C(11)-C(4)	111.5(5)
F(4)-C(11)-C(4)	110.5(6)
F(9)-C(12)-F(7)	109.4(7)
F(9)-C(12)-F(8)	108.0(7)
F(7)-C(12)-F(8)	105.8(7)
F(9)-C(12)-C(7)	112.0(6)
F(7)-C(12)-C(7)	113.4(6)
F(8)-C(12)-C(7)	107.9(6)
O'1-C'1-C'2	129.7(6)
O'1-C'1-C'10	110.5(6)
C'2-C'1-C'10	119.8(6)
C'1-C'2-C'3	121.6(6)
O'2-C'3-C'2	123.8(6)
O'2-C'3-C'13	117.4(6)
C'2-C'3-C'13	118.7(6)
O'3-C'4-C'5	128.2(6)
O'3-C'4-C'11	113.7(6)
C'5-C'4-C'11	118.0(7)
C'4-C'5-C'6	124.2(6)
O'4-C'6-C'5	124.7(6)
O'4-C'6-C'14	116.1(6)
C'5-C'6-C'14	119.1(6)
O'5-C'7-C'8	129.6(6)
O'5-C'7-C'12	110.8(6)
C'8-C'7-C'12	119.6(6)
C'7-C'8-C'9	123.5(6)
O'6-C'9-C'8	124.0(6)
O'6-C'9-C'15	116.3(7)
C'8-C'9-C'15	119.7(6)
F'3-C'10-F'1	105.6(7)
F'3-C'10-F'2	110.0(7)
F'1-C'10-F'2	106.6(7)
F'3-C'10-C'1	112.9(7)
F'1-C'10-C'1	110.5(7)
F'2-C'10-C'1	111.0(6)

F'6-C'11-F'4	106.9(11)
F'6-C'11-F'5	106.4(10)
F'4-C'11-F'5	107.7(10)
F'6-C'11-C'4	110.1(9)
F'4-C'11-C'4	113.5(8)
F'5-C'11-C'4	111.9(8)
F'9-C'12-F'8	108.5(7)
F'9-C'12-F'7	107.5(6)
F'8-C'12-F'7	105.6(6)
F'9-C'12-C'7	112.3(6)
F'8-C'12-C'7	110.2(6)
F'7-C'12-C'7	112.5(6)

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Symmetry transformations used to generate equivalent atoms:

### Table 4. Anisotropic displacement parameters

Table 4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for mo\_roxf02\_0ma\_a. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
Mn(1)	21(1)	28(1)	21(1)	-2(1)	1(1)	2(1)
Mn'1	25(1)	29(1)	21(1)	1(1)	-2(1)	2(1)
O(1)	27(2)	40(2)	33(2)	2(2)	-8(2)	2(2)
O(2)	29(3)	39(2)	26(2)	-7(2)	0(2)	2(2)
O(3)	35(2)	36(2)	30(2)	-3(2)	-5(2)	0(2)
O(4)	27(3)	35(2)	28(2)	-2(2)	4(2)	-3(2)
O(5)	38(2)	28(2)	29(2)	-1(2)	3(2)	1(2)
O(6)	34(2)	41(2)	29(2)	-1(2)	2(2)	3(2)
O'1	33(2)	40(2)	28(2)	0(2)	4(2)	7(2)
O'2	37(3)	41(3)	24(2)	0(2)	-4(2)	5(2)
O'3	36(3)	54(3)	29(2)	-1(2)	4(2)	10(2)
O'4	37(3)	36(3)	32(3)	0(2)	-3(2)	3(2)
O'5	42(2)	25(2)	29(2)	0(2)	-5(2)	3(2)
O'6	38(2)	35(2)	36(3)	-6(2)	-5(2)	1(2)
F(1)	101(4)	78(3)	31(2)	-15(2)	-2(2)	23(3)
F(2)	78(4)	76(3)	87(4)	-40(3)	-16(3)	38(3)
F(3)	129(5)	46(3)	93(4)	-29(3)	19(4)	-39(3)
F(4)	98(4)	49(3)	61(3)	2(2)	-6(3)	33(3)
F(5)	81(3)	55(3)	39(2)	5(2)	9(2)	8(2)
F(6)	92(4)	55(3)	77(3)	21(3)	-19(3)	-35(3)
F(7)	110(5)	61(3)	108(5)	-1(3)	36(4)	25(3)
F(8)	101(4)	90(4)	62(3)	-30(3)	-9(3)	8(3)
F(9)	63(3)	88(4)	130(6)	-58(4)	29(4)	-15(3)
F'1	85(4)	61(3)	115(5)	33(3)	-10(4)	-32(3)
F'2	117(5)	45(2)	37(2)	10(2)	-13(3)	8(3)
F'3	148(6)	48(3)	72(4)	2(3)	8(4)	48(3)
F'4	186(9)	102(5)	130(7)	-73(5)	72(6)	-91(6)
F'5	156(6)	91(4)	47(3)	-22(3)	-9(4)	-22(4)
F'6	301(14)	81(5)	163(8)	-72(6)	-108(9)	108(7)

F'7	83(3)	45(3)	90(4)	32(3)	-24(3)	-8(2)
F'8	40(2)	82(3)	74(3)	38(3)	-5(2)	5(2)
F'9	114(4)	89(4)	35(2)	14(2)	9(3)	49(3)
C(1)	31(3)	29(3)	29(3)	7(2)	4(3)	-1(2)
C(2)	35(3)	30(3)	32(3)	-1(2)	0(3)	6(3)
C(3)	18(3)	40(3)	24(3)	4(2)	6(2)	-3(2)
C(4)	35(3)	26(3)	29(3)	-4(2)	2(3)	6(3)
C(5)	32(3)	33(3)	34(3)	-5(3)	-3(3)	-6(3)
C(6)	18(3)	36(3)	27(3)	-6(3)	5(2)	4(2)
C(7)	29(3)	26(3)	30(3)	-4(2)	-7(2)	5(2)
C(8)	44(4)	32(3)	40(4)	8(3)	2(3)	-4(3)
C(9)	31(3)	34(3)	35(3)	3(3)	-10(3)	0(3)
C(10)	58(5)	44(4)	38(4)	-5(3)	-3(3)	4(3)
C(11)	57(4)	30(3)	39(4)	-2(3)	-4(3)	-2(3)
C(12)	32(3)	33(3)	52(4)	-9(3)	6(3)	-4(3)
C(13)	35(4)	50(4)	25(4)	1(3)	-4(3)	-9(3)
C(14)	33(3)	48(4)	27(3)	-5(3)	1(3)	-4(3)
C(15)	47(4)	48(4)	50(4)	10(4)	5(4)	1(3)
C'1	27(3)	34(3)	31(3)	-7(3)	-4(3)	2(3)
C'2	37(4)	40(3)	39(3)	-6(3)	5(3)	13(3)
C'3	27(3)	45(4)	23(3)	-6(2)	-6(3)	-4(3)
C'4	42(4)	26(3)	33(3)	0(3)	4(3)	7(3)
C'5	42(4)	41(3)	28(3)	0(3)	3(3)	-10(3)
C'6	28(3)	33(3)	23(3)	4(2)	-3(3)	8(2)
C'7	32(3)	30(3)	33(3)	3(3)	9(3)	5(3)
C'8	39(3)	25(3)	58(5)	-5(3)	2(3)	-7(3)
C'9	26(3)	41(4)	42(4)	-12(3)	5(3)	2(3)
C'10	63(5)	37(4)	47(4)	-1(3)	2(4)	6(4)
C'11	109(8)	45(5)	41(5)	-12(4)	1(5)	0(5)
C'12	43(4)	38(3)	40(4)	8(3)	7(3)	7(3)
C'13	36(4)	70(5)	27(4)	-6(3)	-1(3)	-9(3)
C'14	34(4)	51(4)	31(4)	-1(3)	0(3)	9(3)
C'15	46(4)	41(4)	65(5)	-16(4)	-7(4)	-3(3)

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**Table 5. Hydrogen coordinates (  $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for mo\_roxf02\_0ma\_a.**

	x	y	z	U(eq)
H(2)	1276	5926	14527	39
H(5)	5827	6235	15408	40
H(8)	3809	2653	15139	46
H(13A)	764	5034	13293	55
H(13B)	1550	4618	12737	55
H(13C)	1482	5416	12594	55
H(14A)	6599	5470	16596	54
H(14B)	6050	4839	17031	54
H(14C)	5775	5586	17362	54
H(15A)	2993	2612	16582	73
H(15B)	2095	3045	16361	73
H(15C)	2797	3284	17204	73
H'2	8355	8831	12007	47
H'5	3910	8940	13089	45
H'8	6504	12334	12283	49
H'1D	9166	9879	11001	67
H'1E	8416	10243	10321	67
H'1F	8538	9443	10268	67
H'1A	3277	9735	14277	58
H'1B	3871	10365	14641	58
H'1C	4111	9624	15031	58
H'1G	7474	12444	13646	76
H'1H	7974	11786	14069	76
H'1I	7035	12034	14557	76

**Table 6. Torsion angles [°] for mo\_roxf02\_0ma\_a.**

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Mn(1)-O(1)-C(1)-C(2)	7.8(9)
Mn(1)-O(1)-C(1)-C(10)	-172.0(4)
O(1)-C(1)-C(2)-C(3)	-2.2(11)
C(10)-C(1)-C(2)-C(3)	177.6(6)
Mn(1)-O(2)-C(3)-C(2)	-7.3(9)
Mn(1)-O(2)-C(3)-C(13)	171.8(4)
C(1)-C(2)-C(3)-O(2)	1.6(10)
C(1)-C(2)-C(3)-C(13)	-177.4(6)
Mn(1)-O(3)-C(4)-C(5)	15.9(9)
Mn(1)-O(3)-C(4)-C(11)	-164.2(4)
O(3)-C(4)-C(5)-C(6)	-0.5(11)
C(11)-C(4)-C(5)-C(6)	179.7(6)
Mn(1)-O(4)-C(6)-C(5)	-8.0(8)
Mn(1)-O(4)-C(6)-C(14)	172.6(4)
C(4)-C(5)-C(6)-O(4)	-4.2(10)
C(4)-C(5)-C(6)-C(14)	175.2(6)
Mn(1)-O(5)-C(7)-C(8)	-3.4(9)
Mn(1)-O(5)-C(7)-C(12)	177.0(4)
O(5)-C(7)-C(8)-C(9)	2.7(11)
C(12)-C(7)-C(8)-C(9)	-177.7(6)
Mn(1)-O(6)-C(9)-C(8)	-0.8(10)
Mn(1)-O(6)-C(9)-C(15)	179.8(5)
C(7)-C(8)-C(9)-O(6)	-0.4(11)
C(7)-C(8)-C(9)-C(15)	179.0(6)
O(1)-C(1)-C(10)-F(1)	-46.6(9)
C(2)-C(1)-C(10)-F(1)	133.6(7)
O(1)-C(1)-C(10)-F(3)	74.1(8)
C(2)-C(1)-C(10)-F(3)	-105.7(8)
O(1)-C(1)-C(10)-F(2)	-167.6(6)
C(2)-C(1)-C(10)-F(2)	12.6(10)
O(3)-C(4)-C(11)-F(6)	-175.6(6)
C(5)-C(4)-C(11)-F(6)	4.3(10)

O(3)-C(4)-C(11)-F(5)	-52.6(8)
C(5)-C(4)-C(11)-F(5)	127.3(7)
O(3)-C(4)-C(11)-F(4)	65.3(7)
C(5)-C(4)-C(11)-F(4)	-114.8(7)
O(5)-C(7)-C(12)-F(9)	43.6(9)
C(8)-C(7)-C(12)-F(9)	-136.0(8)
O(5)-C(7)-C(12)-F(7)	168.1(6)
C(8)-C(7)-C(12)-F(7)	-11.6(9)
O(5)-C(7)-C(12)-F(8)	-75.2(7)
C(8)-C(7)-C(12)-F(8)	105.2(7)
Mn'1-O'1-C'1-C'2	19.3(10)
Mn'1-O'1-C'1-C'10	-161.3(5)
O'1-C'1-C'2-C'3	-1.0(12)
C'10-C'1-C'2-C'3	179.6(6)
Mn'1-O'2-C'3-C'2	-4.6(9)
Mn'1-O'2-C'3-C'13	175.2(4)
C'1-C'2-C'3-O'2	-6.9(10)
C'1-C'2-C'3-C'13	173.2(6)
Mn'1-O'3-C'4-C'5	14.9(10)
Mn'1-O'3-C'4-C'11	-165.0(5)
O'3-C'4-C'5-C'6	-2.4(12)
C'11-C'4-C'5-C'6	177.5(7)
Mn'1-O'4-C'6-C'5	-8.4(9)
Mn'1-O'4-C'6-C'14	171.7(4)
C'4-C'5-C'6-O'4	-1.8(11)
C'4-C'5-C'6-C'14	178.1(6)
Mn'1-O'5-C'7-C'8	-7.5(10)
Mn'1-O'5-C'7-C'12	174.1(4)
O'5-C'7-C'8-C'9	-3.1(11)
C'12-C'7-C'8-C'9	175.2(6)
Mn'1-O'6-C'9-C'8	1.2(9)
Mn'1-O'6-C'9-C'15	-179.5(5)
C'7-C'8-C'9-O'6	6.2(11)
C'7-C'8-C'9-C'15	-173.0(7)
O'1-C'1-C'10-F'3	173.8(7)
C'2-C'1-C'10-F'3	-6.7(11)

O'1-C'1-C'10-F'1	55.8(8)
C'2-C'1-C'10-F'1	-124.8(8)
O'1-C'1-C'10-F'2	-62.2(9)
C'2-C'1-C'10-F'2	117.3(7)
O'3-C'4-C'11-F'6	75.7(11)
C'5-C'4-C'11-F'6	-104.2(11)
O'3-C'4-C'11-F'4	-164.4(9)
C'5-C'4-C'11-F'4	15.6(12)
O'3-C'4-C'11-F'5	-42.3(11)
C'5-C'4-C'11-F'5	137.7(9)
O'5-C'7-C'12-F'9	-57.8(8)
C'8-C'7-C'12-F'9	123.6(8)
O'5-C'7-C'12-F'8	63.2(8)
C'8-C'7-C'12-F'8	-115.4(7)
O'5-C'7-C'12-F'7	-179.2(6)
C'8-C'7-C'12-F'7	2.2(9)

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Symmetry transformations used to generate equivalent atoms:

**Table 7. Hydrogen bonds for mo\_roxf02\_0ma\_a [ $\text{\AA}$  and  $^\circ$ ].**

D-H...A	d(D-H)	d(H...A)	d(D...A)	$\angle(\text{DHA})$
C(2)-H(2)...F(9)#1	0.95	2.40	3.209(8)	143.3
C(13)-H(13C)...O(1)#2	0.98	2.60	3.372(9)	135.9
C(14)-H(14A)...O(6)#3	0.98	2.64	3.617(8)	174.0
C(14)-H(14C)...O(5)#4	0.98	2.55	3.459(8)	154.0
C'2-H'2...F'8#5	0.95	2.43	3.349(8)	162.1
C'13-H'1D...O'3#5	0.98	2.63	3.544(9)	155.0
C'13-H'1F...O'1#6	0.98	2.66	3.311(8)	124.2
C'14-H'1B...F'2#7	0.98	2.62	3.412(9)	138.5
C'14-H'1C...O'5#8	0.98	2.54	3.499(9)	165.4
C'15-H'1H...F'9#9	0.98	2.63	3.531(11)	152.6

Symmetry transformations used to generate equivalent atoms:

#1  $x-1/2, -y+1, z$     #2  $-x+1/2, y, z-1/2$     #3  $x+1/2, -y+1, z$   
#4  $-x+1, -y+1, z+1/2$     #5  $x+1/2, -y+2, z$     #6  $-x+3/2, y, z-1/2$   
#7  $x-1/2, -y+2, z$     #8  $-x+1, -y+2, z+1/2$     #9  $-x+3/2, y, z+1/2$