X-ray Structure Report

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Experimental

Data Collection

A yellow prismatic crystal of $C_{102}H_{90}O_{18}N_8F_{12}Mn$ having approximate dimensions of 0.20 x 0.40 x 0.15 mm was mounted in a glass capillary. All measurements were made on a Rigaku AFC7R diffractometer with graphite monochromated Mo-Kα radiation and a rotating anode generator.

Cell constants and an orientation matrix for data collection , obtained from a least-squares refinement using the setting angles of 25 carefully centered reflections in the range $30.69 < 2\theta < 34.44°$ corresponded to a primitive monoclinic cell with dimensions:

a = 13.689(4) $\AA$
b = 44.935(6) $\AA$ $\beta = 108.50(2)°$
c = 16.354(4) $\AA$
V = 9539(4) $\AA^3$

For Z = 4 and F.W. = 1998.79, the calculated density is 1.39 g/cm^3. The systematic absences of:

h0l: l $\neq$ 2n
0k0: k $\neq$ 2n

uniquely determine the space group to be:

$P2_1/c$ (#14)

The data were collected at a temperature of -70 $\pm$ 1°C using the ω-2θ scan technique to a maximum 2θ value of 50.0°. Omega scans of several intense reflections, made prior to data collection, had an average width at half-height of 0.42° with a take-off angle of 6.0°. Scans of (1.31 + 0.30 tan θ)° were made at a speed of 16.0°/min (in omega). The weak reflections ($I < 10.0\sigma(I)$) were rescanned (maximum of 5 scans) and the counts were accumulated to ensure good counting statistics. Stationary background counts were recorded on each side of the reflection. The ratio of peak counting time to background counting time was 2:1. The diameter of the incident beam collimator was 6.0 mm and the crystal to detector distance was 400 mm, The computer-controlled slits were set to 9.0 mm (horizontal) and 13.0 mm (vertical).

Data Reduction

Of the 16524 reflections which were collected, 0 were unique ($R_{int} = 0.026$). The intensities of three representative reflection were measured after every 150 reflections. Over the course of data collection, the standards decreased by 0.5%. A linear correction factor was applied to the data to account for this phenomenon.

The linear absorption coefficient, μ, for Mo-Kα radiation is 2.3 cm^{-1}. An empirical absorption correction based on azimuthal scans of several reflections was applied which resulted in transmission factors ranging from 0.92 to 1.00.

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques[2]. Some non-hydrogen atoms were refined anisotropically, while the rest were refined isotropically. Hydrogen atoms were included but not refined. The final cycle of full-matrix least-squares refinement[3] was based on 5503 observed reflections ($I > 3.00\sigma(I)$, $2\theta < 50.03$) and 1034 variable parameters and converged (largest parameter shift was 0.01 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma||Fo| - |Fc||/\Sigma|Fo| = 0.082$$

$$R_w = \sqrt{\Sigma w(|Fo| - |Fc|)^2/\Sigma wFo^2} = 0.122$$

$$R1 = \Sigma||Fo| - |Fc||/\Sigma|Fo| = 0.082 \quad for \quad I > 3.0\sigma(I) \quad data$$

The standard deviation of an observation of unit weight[4] was 1.31. The weighting scheme was based on counting statistics and included a factor (p = 0.171) to downweight the intense reflections. Plots of $\Sigma w(|Fo| - |Fc|)^2$ versus $|Fo|$, reflection order in data collection, sin θ/λ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 1.27 and -0.64 $e^-/\mathring{A}^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5] . Anomalous dispersion effects were included in Fcalc[6]; the values for Δf' and Δf" were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbel[8]. All calculations were performed using the teXsan[9] crystallographic software package of Molecular Structure Corporation.

References

(1) SIR92: Altomare, A., Burla, M.C., Camalli, M., Cascarano, M., Giacovazzo, C., Guagliardi, A., Polidori, G., (1994). J. Appl. Cryst. 27, 435.

(2) DIRDIF94: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M. (1994). The DIRDIF-94 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(3) Least-Squares:

Function minimized: $\Sigma w(|Fo| - |Fc|)^2$

where w = $\frac{1}{\sigma^2(Fo)} = [\sigma_c^2(Fo) + \frac{p^2}{4}Fo^2]^{-1}$

$\sigma_c(Fo)$ = e.s.d. based on counting statistics

p = p-factor

(4) Standard deviation of an observation of unit weight:

$$\sqrt{\Sigma w(|Fo| - |Fc|)^2/(No - Nv)}$$

where: No = number of observations

Nv = number of variables

(5) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(6) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(7) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(8) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(9) teXsan: Crystal Structure Analysis Package, Molecular Structure Corporation (1985 & 1999).

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{102}H_{90}O_{18}N_8F_{12}Mn$
Formula Weight	1998.79
Crystal Color, Habit	yellow, prismatic
Crystal Dimensions	0.20 X 0.40 X 0.15 mm
Crystal System	monoclinic
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2θ range)	25 (30.7 - 34.4°)
Omega Scan Peak Width at Half-height	0.42°
Lattice Parameters	a = 13.689(4) $\AA$ b = 44.935(6) $\AA$ c = 16.354(4) $\AA$ β = 108.50(2)° V = 9539(4) $\AA^3$
Space Group	$P2_1/c$ (#14)
Z value	4
D_{calc}	1.392 g/cm^3
F_{000}	4140.00
μ(MoKα)	2.35 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC7R (rotating anode)
Radiation	MoKα (λ = 0.71069 $\AA$) graphite monochromated
Attenuator	Zr foil (factor = 8.73)

Temperature	-70.0 °C
Collimator Size	6.0 mm
Take-off Angle	6.0°
Detector Aperture	9.0 mm horizontal 13.0 mm vertical
Crystal to Detector Distance	400 mm
Scan Type	ω-2θ
Scan Rate	16.0°/min (in ω) (up to 5 scans)
Scan Width	(1.31 + 0.30 tan θ)°
$2\theta_{max}$	50.0°
No. of Reflections Measured	Total: 16524 Unique: 0 (R_{int} = 0.026)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.9247 - 0.9988) Decay (0.47% decline)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma w(\|Fo\| - \|Fc\|)^2$
Least Squares Weights	$w = \frac{1}{\sigma^2(Fo)} = [\sigma_c^2(Fo) + \frac{p^2}{4}Fo^2]^{-1}$
p-factor	0.1710
Anomalous Dispersion	All non-hydrogen atoms
No. of Observations (I>3.00σ(I), 2θ<50.03°)	5503
No. Variables	1034
Reflection/Parameter Ratio	5.32
Residuals: R; Rw	0.082 ; 0.122
Residuals: R1	0.082

No. of Reflections to calc R1	5503
Goodness of Fit Indicator	1.31
Max Shift/Error in Final Cycle	0.011
Maximum peak in Final Diff. Map	1.27 $e^-/\mathring{A}^3$
Minimum peak in Final Diff. Map	-0.64 $e^-/\mathring{A}^3$

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
Mn(1)	0.8382(1)	0.19303(4)	0.7328(1)	2.68(4)	1.0000
F(1)	1.0685	0.2357	0.5425	6.2131	0.5000
F(2)	1.0118	0.2373	0.5031	5.4804	0.4700
F(3)	0.9175	0.2559	0.5158	10.4081	0.6500
F(4)	0.9476	0.2680	0.5755	6.2510	0.4800
F(5)	1.0349	0.2632	0.6359	7.4464	0.4500
F(6)	1.0839	0.2492	0.6347	6.1918	0.4500
F(7)	1.0157	0.1374	0.5183	3.4204	0.3000
F(8)	0.9463	0.1350	0.4825	5.2277	0.5000
F(9)	0.8886	0.1320	0.4797	5.7394	0.2500
F(10)	0.8741	0.1129	0.5555	6.0481	0.8000
F(11)	0.9483	0.1084	0.5995	17.6761	0.3000
F(12)	1.0230	0.1179	0.6256	4.7864	0.5000
F(13)	1.0464	0.1259	0.5879	7.9138	0.3500
F(14)	0.7030	0.2724	0.8561	6.5605	0.3200
F(15)	0.6464	0.2692	0.8076	3.3367	0.3600
F(16)	0.5903	0.2562	0.7968	6.6426	0.4000
F(17)	0.5720	0.2450	0.8737	5.3477	0.4000
F(18)	0.6180	0.2406	0.9231	5.9083	0.5500
F(19)	0.7162	0.2534	0.9450	17.4242	0.3700
F(20)	0.7396	0.2628	0.9202	7.2727	0.6000
F(21)	0.6190	0.1195	0.7758	6.3860	0.3000
F(22)	0.6980	0.1138	0.8521	10.8992	0.7000
F(23)	0.7015	0.1277	0.9160	15.9351	0.4000

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
F(24)	0.6100	0.1345	0.8947	5.2017	0.4000
F(25)	0.5549	0.1428	0.8563	4.5740	0.4000
F(26)	0.5536	0.1368	0.7612	17.6421	0.4000
F(27)	0.5850	0.1269	0.7465	5.1432	0.4000
O(1)	1.3598(6)	0.1424(2)	1.5192(5)	2.6(2)	1.0000
O(2)	1.1798(5)	0.1402(2)	1.4472(4)	2.3(2)	1.0000
O(3)	0.9604(5)	0.1281(2)	1.1563(5)	2.4(2)	1.0000
O(4)	0.9913(6)	0.1261(2)	1.0232(5)	2.6(2)	1.0000
O(5)	1.2971(5)	0.1287(2)	0.9424(4)	2.4(2)	1.0000
O(6)	1.4789(5)	0.1262(2)	1.0092(5)	2.6(2)	1.0000
O(7)	1.6960(6)	0.1313(2)	1.3021(5)	2.6(2)	1.0000
O(8)	1.6649(5)	0.1353(2)	1.4372(5)	2.6(2)	1.0000
O(9)	0.9046(6)	0.2229(2)	0.6629(5)	3.6(2)	1.0000
O(10)	0.8849(7)	0.1588(2)	0.6616(6)	3.9(2)	1.0000
O(11)	0.7788(6)	0.2235(2)	0.8050(5)	3.2(2)	1.0000
O(12)	0.7708(7)	0.1599(2)	0.7930(6)	3.8(2)	1.0000
O(13)	1.321(1)	0.1862(2)	1.2927(8)	7.4(4)	1.0000
O(14)	1.3500(9)	0.1879(2)	1.1683(7)	5.9(3)	1.0000
O(15)	1.3743	0.0063	1.2455	7.7(3)	1.0000
O(16)	1.3907	-0.0414	1.2774	6.7(3)	1.0000
O(17)	1.3219	0.2509	1.3732	30.0(9)	1.0000
O(18)	1.2303	0.2921	1.2762	29.0(9)	1.0000
N(1)	1.5330(8)	0.2196(2)	1.5416(7)	3.5(3)	1.0000
N(2)	1.6826(7)	0.1944(2)	1.6267(6)	2.8(2)	1.0000

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
N(3)	1.0074(8)	0.2157(2)	1.3170(7)	3.8(3)	1.0000
N(4)	0.8650(8)	0.1865(2)	1.3158(8)	4.3(3)	1.0000
N(5)	0.9887(7)	0.1866(2)	0.8395(6)	2.9(2)	1.0000
N(6)	1.1438(8)	0.2096(2)	0.9329(7)	4.3(3)	1.0000
N(7)	1.7646(10)	0.1779(3)	1.0828(9)	5.7(4)	1.0000
N(8)	1.6590(9)	0.2090(2)	1.1321(8)	4.6(3)	1.0000
C(1)	1.5127(9)	0.1395(2)	1.4773(7)	2.5(3)	1.0000
C(2)	1.5712(8)	0.1233(3)	1.4353(7)	2.3(3)	1.0000
C(3)	1.5415(8)	0.0956(2)	1.3984(7)	2.0(3)	1.0000
C(4)	1.4499(9)	0.0839(2)	1.4038(7)	2.5(3)	1.0000
C(5)	1.3866(8)	0.0983(2)	1.4427(7)	2.2(3)	1.0000
C(6)	1.4174(8)	0.1267(3)	1.4772(7)	2.3(3)	1.0000
C(7)	1.2839(8)	0.0863(2)	1.4467(7)	2.1(3)	1.0000
C(8)	1.2724(9)	0.1575(3)	1.4654(8)	2.8(3)	1.0000
C(9)	1.1524(8)	0.1236(2)	1.3702(7)	2.3(3)	1.0000
C(10)	1.0730(8)	0.1350(2)	1.3004(8)	2.4(3)	1.0000
C(11)	1.0423(8)	0.1179(3)	1.2253(8)	2.5(3)	1.0000
C(12)	1.0897(8)	0.0909(2)	1.2187(7)	2.1(3)	1.0000
C(13)	1.1678(8)	0.0812(2)	1.2905(7)	2.2(3)	1.0000
C(14)	1.1998(8)	0.0968(2)	1.3685(7)	2.1(3)	1.0000
C(15)	1.0589(8)	0.0746(2)	1.1316(7)	2.4(3)	1.0000
C(16)	0.9844(8)	0.1442(2)	1.0916(7)	2.3(3)	1.0000
C(17)	1.0874(8)	0.1140(2)	1.0306(7)	2.3(3)	1.0000
C(18)	1.1487(8)	0.1281(2)	0.9895(7)	2.1(3)	1.0000

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
C(19)	1.2420(8)	0.1155(3)	0.9917(7)	2.6(3)	1.0000
C(20)	1.2752(8)	0.0887(2)	1.0342(7)	2.2(3)	1.0000
C(21)	1.2154(8)	0.0759(2)	1.0784(6)	1.9(2)	1.0000
C(22)	1.1207(8)	0.0883(3)	1.0781(7)	2.4(3)	1.0000
C(23)	1.3778(8)	0.0747(2)	1.0349(7)	2.0(3)	1.0000
C(24)	1.3893(9)	0.1447(3)	0.9874(8)	3.0(3)	1.0000
C(25)	1.5100(8)	0.1142(2)	1.0914(7)	2.3(3)	1.0000
C(26)	1.5872(8)	0.1289(2)	1.1554(7)	2.3(3)	1.0000
C(27)	1.6164(8)	0.1167(2)	1.2387(7)	2.2(3)	1.0000
C(28)	1.5720(8)	0.0907(2)	1.2595(7)	2.1(3)	1.0000
C(29)	1.4956(8)	0.0767(2)	1.1915(7)	2.2(3)	1.0000
C(30)	1.4623(8)	0.0885(3)	1.1081(7)	2.2(3)	1.0000
C(31)	1.6064(8)	0.0796(2)	1.3530(7)	2.0(3)	1.0000
C(32)	1.6675(9)	0.1499(2)	1.3612(8)	2.9(3)	1.0000
C(33)	1.5507(8)	0.1677(2)	1.5207(7)	2.4(3)	1.0000
C(34)	1.4981(9)	0.1944(3)	1.5009(7)	3.0(3)	1.0000
C(35)	1.6235(9)	0.2184(3)	1.6025(8)	3.0(3)	1.0000
C(36)	1.6446(9)	0.1691(3)	1.5849(8)	2.9(3)	1.0000
C(37)	1.0167(8)	0.1626(3)	1.3063(8)	2.6(3)	1.0000
C(38)	1.0604(9)	0.1899(3)	1.3114(8)	3.1(3)	1.0000
C(39)	0.9141(10)	0.2124(3)	1.3196(10)	4.2(4)	1.0000
C(40)	0.9168(9)	0.1622(3)	1.3083(8)	3.2(3)	1.0000
C(41)	1.1123(9)	0.1570(2)	0.9428(7)	2.4(3)	1.0000
C(42)	1.0199(9)	0.1604(3)	0.8782(8)	3.0(3)	1.0000

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
C(43)	1.0540(10)	0.2098(3)	0.8697(9)	3.7(3)	1.0000
C(44)	1.1721(9)	0.1827(3)	0.9679(8)	3.3(3)	1.0000
C(45)	1.6383(8)	0.1561(3)	1.1362(7)	2.5(3)	1.0000
C(46)	1.717(1)	0.1541(3)	1.1015(10)	4.5(4)	1.0000
C(47)	1.732(1)	0.2039(3)	1.1025(9)	4.1(4)	1.0000
C(48)	1.613(1)	0.1840(3)	1.1499(10)	4.3(4)	1.0000
C(49)	1.2840(8)	0.0522(2)	1.4610(7)	2.4(3)	1.0000
C(50)	1.3570(9)	0.0441(2)	1.5514(8)	2.7(3)	1.0000
C(51)	1.3253(9)	0.0573(3)	1.6236(8)	2.9(3)	1.0000
C(52)	1.382(1)	0.0808(3)	1.6705(9)	4.0(4)	1.0000
C(53)	1.355(1)	0.0933(3)	1.7384(10)	5.0(4)	1.0000
C(54)	1.271(1)	0.0822(4)	1.7593(9)	5.3(4)	1.0000
C(55)	1.214(1)	0.0599(3)	1.7120(9)	4.6(4)	1.0000
C(56)	1.2410(10)	0.0475(3)	1.6427(8)	3.5(3)	1.0000
C(57)	1.0679(9)	0.0407(2)	1.1402(7)	2.6(3)	1.0000
C(58)	0.9960(9)	0.0273(3)	1.1857(7)	2.8(3)	1.0000
C(59)	1.0104(8)	-0.0059(3)	1.1991(8)	2.8(3)	1.0000
C(60)	1.041(1)	-0.0180(3)	1.2815(9)	4.0(4)	1.0000
C(61)	1.056(1)	-0.0484(3)	1.2950(10)	5.0(4)	1.0000
C(62)	1.039(1)	-0.0675(3)	1.225(1)	4.7(4)	1.0000
C(63)	1.008(1)	-0.0558(3)	1.1425(8)	4.2(4)	1.0000
C(64)	0.995(1)	-0.0256(3)	1.1275(8)	4.0(4)	1.0000
C(65)	1.3735(9)	0.0405(3)	1.0366(7)	2.8(3)	1.0000
C(66)	1.2934(9)	0.0273(3)	0.9578(7)	2.9(3)	1.0000

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
C(67)	1.2772(9)	-0.0053(3)	0.9650(7)	2.8(3)	1.0000
C(68)	1.2297(9)	-0.0163(3)	1.0218(7)	2.8(3)	1.0000
C(69)	1.216(1)	-0.0466(3)	1.0307(9)	4.1(4)	1.0000
C(70)	1.250(1)	-0.0667(3)	0.9827(10)	4.9(4)	1.0000
C(71)	1.298(1)	-0.0562(3)	0.9270(10)	4.9(4)	1.0000
C(72)	1.3141(9)	-0.0258(3)	0.9193(8)	3.2(3)	1.0000
C(73)	1.6072(8)	0.0454(2)	1.3607(7)	2.1(3)	1.0000
C(74)	1.6842(8)	0.0312(2)	1.3228(7)	2.5(3)	1.0000
C(75)	1.7954(9)	0.0410(2)	1.3684(8)	2.7(3)	1.0000
C(76)	1.8436(9)	0.0617(3)	1.3318(8)	3.1(3)	1.0000
C(77)	1.941(1)	0.0715(3)	1.3733(10)	3.9(4)	1.0000
C(78)	1.9942(10)	0.0602(3)	1.4541(9)	4.0(4)	1.0000
C(79)	1.9495(10)	0.0386(3)	1.4887(8)	3.4(3)	1.0000
C(80)	1.8513(9)	0.0294(3)	1.4497(8)	2.8(3)	1.0000
C(81)	0.947(1)	0.2159(3)	0.6093(9)	4.0(4)	1.0000
C(82)	0.960(1)	0.1882(3)	0.5770(8)	4.5(4)	1.0000
C(83)	0.926(1)	0.1618(3)	0.6034(8)	3.7(3)	1.0000
C(84)	0.9947	0.2429	0.5762	5.3(3)	1.0000
C(85)	0.9499	0.1328	0.5641	5.7(4)	1.0000
C(86)	0.7073(10)	0.2190(3)	0.8354(8)	3.5(3)	1.0000
C(87)	0.665(1)	0.1908(4)	0.8452(9)	5.0(4)	1.0000
C(88)	0.700(1)	0.1640(3)	0.8208(9)	4.5(4)	1.0000
C(89)	0.6625	0.2472	0.8637	6.4(4)	1.0000
C(90)	0.6388	0.1370	0.8307	10.3(6)	1.0000

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
C(91)	1.333(1)	0.1402(3)	1.2244(9)	4.5(4)	1.0000
C(92)	1.334(1)	0.1734(4)	1.2309(9)	4.4(4)	1.0000
C(93)	1.342(2)	0.2224(5)	1.170(2)	11.4(9)	1.0000
C(94)	1.361(2)	0.2358(6)	1.103(2)	14(1)	1.0000
C(95)	1.4798	-0.0239	1.1838	6.5(4)	1.0000
C(96)	1.4106	-0.0164	1.2369	6.1(4)	1.0000
C(97)	1.3549	-0.0408	1.3277	12.1(7)	1.0000
C(98)	1.3213	-0.0686	1.3743	7.4(5)	1.0000
C(99)	1.3910	0.3025	1.3528	11.6(7)	1.0000
C(100)	1.3245	0.2819	1.3438	31.1(7)	1.0000
C(101)	1.2197	0.3302	1.2456	13.4(8)	1.0000
C(102)	1.2443	0.3331	1.1621	25.5(8)	1.0000
H(1)	1.4259	0.0651	1.3779	2.6	1.0000
H(2)	1.2728	0.0949	1.4967	2.8	1.0000
H(3)	1.2654	0.1766	1.4910	3.1	1.0000
H(4)	1.2848	0.1623	1.4111	3.1	1.0000
H(5)	1.2017	0.0625	1.2882	3.1	1.0000
H(6)	0.9852	0.0785	1.0999	2.7	1.0000
H(7)	1.0506	0.1547	1.1158	3.2	1.0000
H(8)	0.9347	0.1602	1.0678	3.2	1.0000
H(9)	1.2418	0.0586	1.1132	2.2	1.0000
H(10)	1.3887	0.0798	0.9806	2.4	1.0000
H(11)	1.3817	0.1529	1.0389	3.7	1.0000
H(12)	1.3966	0.1607	0.9513	3.7	1.0000

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
H(13)	1.4677	0.0578	1.1991	2.7	1.0000
H(14)	1.6795	0.0853	1.3812	2.6	1.0000
H(15)	1.7156	0.1667	1.3790	3.4	1.0000
H(16)	1.6006	0.1588	1.3349	3.4	1.0000
H(17)	1.4301	0.1935	1.4544	3.3	1.0000
H(18)	1.6503	0.2379	1.6336	3.7	1.0000
H(19)	1.6837	0.1498	1.6012	3.6	1.0000
H(20)	1.1309	0.1917	1.3076	3.9	1.0000
H(21)	0.8731	0.2304	1.3225	4.7	1.0000
H(22)	0.8793	0.1428	1.3052	4.0	1.0000
H(23)	0.9755	0.1428	0.8577	3.3	1.0000
H(24)	1.0303	0.2294	0.8420	4.4	1.0000
H(25)	1.2377	0.1808	1.0169	5.2	1.0000
H(26)	1.7424	0.1336	1.0920	4.8	1.0000
H(27)	1.7708	0.2216	1.0907	5.6	1.0000
H(28)	1.5505	0.1863	1.1661	5.3	1.0000
H(29)	1.3041	0.0414	1.4169	2.8	1.0000
H(30)	1.2167	0.0446	1.4577	2.8	1.0000
H(31)	1.4253	0.0506	1.5509	2.9	1.0000
H(32)	1.3611	0.0226	1.5554	2.9	1.0000
H(33)	1.4434	0.0884	1.6548	5.3	1.0000
H(34)	1.3991	0.1094	1.7731	6.4	1.0000
H(35)	1.2518	0.0932	1.8055	5.8	1.0000
H(36)	1.1516	0.0524	1.7254	5.5	1.0000

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
H(37)	1.1979	0.0310	1.6043	4.3	1.0000
H(38)	1.1373	0.0356	1.1695	2.9	1.0000
H(39)	1.0529	0.0318	1.0808	2.9	1.0000
H(40)	1.0043	0.0366	1.2384	4.3	1.0000
H(41)	0.9221	0.0310	1.1494	4.3	1.0000
H(42)	1.0511	-0.0049	1.3296	4.4	1.0000
H(43)	1.0854	-0.0572	1.3562	6.4	1.0000
H(44)	1.0509	-0.0890	1.2324	5.1	1.0000
H(45)	0.9897	-0.0691	1.0895	5.6	1.0000
H(46)	0.9719	-0.0164	1.0655	5.8	1.0000
H(47)	1.3609	0.0338	1.0881	2.6	1.0000
H(48)	1.4411	0.0322	1.0392	2.6	1.0000
H(49)	1.2298	0.0377	0.9527	3.0	1.0000
H(50)	1.3130	0.0318	0.9087	3.0	1.0000
H(51)	1.2038	-0.0022	1.0553	3.9	1.0000
H(52)	1.1801	-0.0541	1.0700	5.4	1.0000
H(53)	1.2381	-0.0890	0.9846	5.8	1.0000
H(54)	1.3267	-0.0700	0.8929	4.8	1.0000
H(55)	1.3525	-0.0192	0.8806	3.8	1.0000
H(56)	1.5380	0.0380	1.3345	3.3	1.0000
H(57)	1.6246	0.0396	1.4227	3.3	1.0000
H(58)	1.6636	0.0378	1.2638	3.4	1.0000
H(59)	1.6783	0.0104	1.3243	3.4	1.0000
H(60)	1.8075	0.0703	1.2749	3.9	1.0000

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
H(61)	1.9731	0.0869	1.3480	4.4	1.0000
H(62)	2.0656	0.0663	1.4855	4.3	1.0000
H(63)	1.9897	0.0300	1.5447	4.5	1.0000
H(64)	1.8185	0.0145	1.4770	3.4	1.0000
H(65)	0.9882	0.1872	0.5272	5.7	1.0000
H(66)	0.5991	0.1924	0.8659	6.7	1.0000

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Mn(1)	0.034(1)	0.031(1)	0.034(1)	-0.0001(9)	0.0081(8)	0.0005(9)
O(1)	0.037(5)	0.032(5)	0.034(5)	0.002(4)	0.014(4)	-0.004(4)
O(2)	0.027(4)	0.032(5)	0.026(4)	-0.001(3)	0.003(3)	-0.005(4)
O(3)	0.026(4)	0.033(5)	0.031(5)	0.005(3)	0.006(4)	0.010(4)
O(4)	0.036(5)	0.031(5)	0.032(5)	0.007(4)	0.010(4)	0.006(4)
O(5)	0.034(4)	0.034(5)	0.023(4)	-0.005(4)	0.012(4)	0.007(4)
O(6)	0.028(4)	0.037(5)	0.035(5)	-0.005(4)	0.009(4)	0.002(4)
O(7)	0.033(4)	0.024(5)	0.040(5)	0.000(3)	0.011(4)	-0.001(4)
O(8)	0.025(4)	0.043(5)	0.026(5)	-0.009(4)	0.003(3)	-0.001(4)
O(9)	0.052(6)	0.045(6)	0.039(6)	-0.003(4)	0.012(4)	0.002(4)
O(10)	0.052(6)	0.051(6)	0.048(6)	0.005(4)	0.019(5)	-0.004(5)
O(11)	0.036(5)	0.041(5)	0.048(6)	-0.006(4)	0.015(4)	-0.001(4)
O(12)	0.049(6)	0.044(6)	0.052(6)	0.000(4)	0.016(5)	-0.001(5)
O(13)	0.16(1)	0.058(8)	0.074(9)	-0.005(7)	0.061(9)	-0.010(6)
O(14)	0.121(10)	0.056(8)	0.059(7)	-0.008(6)	0.047(7)	0.009(6)
N(1)	0.056(7)	0.022(6)	0.047(7)	0.001(5)	0.006(6)	-0.004(5)
N(2)	0.040(6)	0.025(6)	0.037(6)	-0.005(5)	0.007(5)	-0.010(5)
N(3)	0.050(7)	0.018(6)	0.075(8)	0.000(5)	0.019(6)	-0.011(5)
N(4)	0.047(7)	0.045(8)	0.079(9)	0.021(6)	0.029(6)	0.005(6)
N(5)	0.035(6)	0.035(7)	0.034(6)	0.007(5)	0.002(5)	0.004(5)
N(6)	0.040(7)	0.033(7)	0.071(8)	-0.001(5)	-0.011(6)	0.007(6)
N(7)	0.076(9)	0.046(8)	0.13(1)	-0.005(7)	0.079(9)	0.015(8)
N(8)	0.057(8)	0.037(7)	0.10(1)	0.003(6)	0.046(8)	0.004(7)
C(1)	0.044(7)	0.028(7)	0.024(6)	0.000(6)	0.012(5)	-0.003(5)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(2)	0.024(6)	0.031(7)	0.028(7)	-0.007(5)	0.005(5)	-0.006(5)
C(3)	0.032(7)	0.019(7)	0.026(7)	0.003(5)	0.010(5)	0.000(5)
C(4)	0.035(7)	0.026(7)	0.034(7)	-0.002(5)	0.009(5)	0.004(5)
C(5)	0.034(7)	0.022(7)	0.023(6)	0.009(5)	0.005(5)	-0.001(5)
C(6)	0.035(7)	0.033(7)	0.022(6)	0.001(5)	0.011(5)	-0.004(5)
C(7)	0.018(6)	0.032(7)	0.029(7)	-0.005(5)	0.009(5)	-0.001(5)
C(8)	0.034(7)	0.025(7)	0.046(8)	0.013(5)	0.009(6)	0.002(6)
C(9)	0.034(7)	0.029(7)	0.024(6)	-0.012(5)	0.010(5)	-0.005(5)
C(10)	0.027(6)	0.027(7)	0.037(7)	-0.006(5)	0.008(5)	0.000(6)
C(11)	0.020(6)	0.037(8)	0.038(8)	0.003(5)	0.010(5)	0.004(6)
C(12)	0.025(6)	0.034(7)	0.024(6)	0.002(5)	0.015(5)	0.001(5)
C(13)	0.027(6)	0.017(6)	0.046(8)	0.003(5)	0.018(6)	0.005(5)
C(14)	0.022(6)	0.029(7)	0.032(7)	-0.002(5)	0.011(5)	0.001(6)
C(15)	0.030(7)	0.031(7)	0.027(7)	-0.003(5)	0.006(5)	0.002(5)
C(16)	0.042(7)	0.017(6)	0.033(7)	0.010(5)	0.018(6)	0.006(5)
C(17)	0.031(7)	0.028(7)	0.025(7)	0.001(5)	0.004(5)	-0.008(5)
C(18)	0.026(6)	0.026(7)	0.032(7)	0.003(5)	0.013(5)	-0.004(5)
C(19)	0.026(6)	0.034(8)	0.031(7)	-0.004(5)	-0.003(5)	0.009(6)
C(20)	0.021(6)	0.030(7)	0.034(7)	0.007(5)	0.010(5)	0.012(6)
C(21)	0.026(6)	0.025(6)	0.017(6)	-0.002(5)	0.001(5)	0.000(5)
C(22)	0.037(7)	0.035(7)	0.015(6)	-0.001(5)	0.002(5)	-0.001(5)
C(23)	0.040(7)	0.013(6)	0.024(6)	-0.005(5)	0.014(5)	-0.008(5)
C(24)	0.034(7)	0.023(7)	0.054(9)	0.005(5)	0.013(6)	0.015(6)
C(25)	0.031(7)	0.031(7)	0.033(7)	0.007(5)	0.018(5)	0.011(6)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(26)	0.024(6)	0.028(7)	0.036(7)	0.006(5)	0.013(5)	-0.003(6)
C(27)	0.024(6)	0.029(7)	0.030(7)	0.010(5)	0.007(5)	0.009(6)
C(28)	0.027(6)	0.033(7)	0.021(6)	-0.006(5)	0.008(5)	-0.003(5)
C(29)	0.029(6)	0.015(6)	0.039(8)	0.001(5)	0.011(5)	-0.001(5)
C(30)	0.023(6)	0.034(7)	0.023(6)	0.007(5)	0.005(5)	0.004(5)
C(31)	0.025(6)	0.028(7)	0.026(6)	-0.002(5)	0.009(5)	0.001(5)
C(32)	0.037(7)	0.027(7)	0.048(8)	-0.001(5)	0.017(6)	-0.002(6)
C(33)	0.025(6)	0.026(7)	0.039(8)	0.003(5)	0.011(5)	-0.004(6)
C(34)	0.047(7)	0.041(8)	0.017(6)	-0.003(6)	-0.002(5)	0.009(6)
C(35)	0.035(7)	0.027(7)	0.041(8)	0.003(6)	-0.003(6)	-0.005(6)
C(36)	0.046(8)	0.037(8)	0.031(7)	0.008(6)	0.016(6)	0.004(6)
C(37)	0.025(6)	0.027(7)	0.048(8)	-0.005(5)	0.012(6)	-0.010(6)
C(38)	0.042(7)	0.026(7)	0.049(8)	0.003(6)	0.014(6)	0.000(6)
C(39)	0.034(8)	0.021(8)	0.10(1)	0.007(6)	0.020(8)	-0.005(7)
C(40)	0.035(7)	0.029(8)	0.064(9)	0.002(6)	0.024(7)	-0.007(6)
C(41)	0.035(7)	0.025(7)	0.030(7)	0.000(5)	0.009(5)	-0.003(6)
C(42)	0.044(8)	0.031(7)	0.035(8)	0.009(6)	0.005(6)	0.008(6)
C(43)	0.046(8)	0.029(8)	0.065(10)	0.010(6)	0.015(7)	0.023(7)
C(44)	0.035(7)	0.028(7)	0.051(9)	0.007(6)	-0.004(6)	0.003(6)
C(45)	0.030(7)	0.027(7)	0.037(7)	-0.004(5)	0.010(5)	0.005(6)
C(46)	0.061(9)	0.031(8)	0.09(1)	0.005(7)	0.048(9)	0.005(8)
C(47)	0.055(9)	0.026(8)	0.08(1)	-0.005(7)	0.023(8)	0.022(7)
C(48)	0.053(8)	0.038(9)	0.09(1)	-0.001(7)	0.058(9)	0.009(8)
C(49)	0.033(7)	0.025(7)	0.036(7)	-0.002(5)	0.016(5)	0.003(5)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(50)	0.046(7)	0.021(7)	0.039(8)	0.003(5)	0.021(6)	0.007(6)
C(51)	0.039(7)	0.030(7)	0.033(8)	-0.001(6)	-0.001(6)	0.008(6)
C(52)	0.057(9)	0.049(9)	0.039(9)	-0.005(7)	0.008(7)	0.009(7)
C(53)	0.08(1)	0.049(10)	0.06(1)	-0.017(8)	0.006(9)	-0.002(8)
C(54)	0.08(1)	0.07(1)	0.043(10)	0.009(9)	0.004(8)	-0.018(8)
C(55)	0.045(9)	0.08(1)	0.055(10)	0.000(8)	0.021(7)	-0.010(9)
C(56)	0.046(8)	0.039(8)	0.047(8)	0.012(6)	0.016(7)	-0.003(6)
C(57)	0.041(7)	0.030(7)	0.031(7)	0.005(5)	0.015(6)	0.007(6)
C(58)	0.039(7)	0.038(8)	0.030(7)	-0.007(6)	0.011(6)	-0.009(6)
C(59)	0.021(6)	0.048(8)	0.041(8)	-0.004(5)	0.016(6)	0.003(6)
C(60)	0.07(1)	0.037(8)	0.046(9)	0.003(7)	0.025(8)	-0.003(7)
C(61)	0.09(1)	0.05(1)	0.06(1)	0.007(8)	0.039(9)	0.012(8)
C(62)	0.07(1)	0.039(9)	0.07(1)	0.010(8)	0.029(9)	0.010(8)
C(63)	0.08(1)	0.038(9)	0.032(8)	-0.009(7)	-0.003(7)	-0.019(7)
C(64)	0.070(10)	0.036(9)	0.040(8)	-0.008(7)	0.007(7)	-0.010(7)
C(65)	0.043(8)	0.029(7)	0.037(8)	0.000(6)	0.015(6)	0.003(6)
C(66)	0.055(8)	0.025(7)	0.033(7)	-0.011(6)	0.020(6)	-0.004(6)
C(67)	0.041(7)	0.029(7)	0.028(7)	-0.001(5)	0.003(6)	0.002(6)
C(68)	0.048(8)	0.031(8)	0.024(7)	0.005(6)	0.006(6)	-0.010(5)
C(69)	0.059(9)	0.036(9)	0.07(1)	-0.015(7)	0.030(8)	-0.002(8)
C(70)	0.08(1)	0.044(10)	0.048(10)	-0.004(8)	0.008(9)	0.009(8)
C(71)	0.063(10)	0.045(10)	0.07(1)	0.013(8)	0.004(8)	-0.030(8)
C(72)	0.037(7)	0.043(9)	0.041(8)	0.003(6)	0.010(6)	-0.018(7)
C(73)	0.031(6)	0.019(6)	0.030(7)	-0.001(5)	0.007(5)	0.001(5)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(74)	0.033(7)	0.033(7)	0.028(7)	0.008(5)	0.009(5)	0.004(5)
C(75)	0.054(8)	0.014(6)	0.045(8)	0.005(5)	0.028(7)	0.003(6)
C(76)	0.044(8)	0.033(8)	0.043(8)	0.004(6)	0.020(6)	0.010(6)
C(77)	0.046(9)	0.039(9)	0.07(1)	-0.003(6)	0.031(8)	0.009(7)
C(78)	0.043(8)	0.052(10)	0.056(10)	0.001(7)	0.014(7)	-0.011(8)
C(79)	0.048(9)	0.036(8)	0.044(8)	0.010(6)	0.015(7)	0.005(6)
C(80)	0.040(8)	0.039(8)	0.031(7)	-0.002(6)	0.018(6)	0.003(6)
C(81)	0.062(9)	0.053(10)	0.036(8)	0.002(7)	0.015(7)	-0.008(7)
C(82)	0.09(1)	0.05(1)	0.039(9)	0.012(8)	0.042(8)	0.005(7)
C(83)	0.067(10)	0.039(9)	0.030(8)	0.008(7)	0.008(7)	-0.002(6)
C(86)	0.035(7)	0.07(1)	0.035(8)	-0.003(7)	0.014(6)	-0.009(7)
C(87)	0.08(1)	0.07(1)	0.06(1)	-0.027(9)	0.045(9)	-0.001(9)
C(88)	0.08(1)	0.039(9)	0.049(10)	-0.029(8)	0.019(9)	-0.001(7)
C(91)	0.063(9)	0.031(8)	0.07(1)	-0.002(7)	0.011(8)	0.014(8)
C(92)	0.069(10)	0.07(1)	0.021(7)	0.001(9)	0.004(6)	-0.005(8)
C(93)	0.27(3)	0.06(2)	0.13(2)	0.00(2)	0.10(2)	-0.01(1)
C(94)	0.24(3)	0.19(3)	0.12(2)	-0.10(2)	0.07(2)	0.03(2)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table 3. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
Mn(1)	O(9)	2.142(8)	Mn(1)	O(10)	2.143(9)
Mn(1)	O(11)	2.130(8)	Mn(1)	O(12)	2.148(9)
Mn(1)	N(2)$^{1)}$	2.282(10)	Mn(1)	N(5)	2.257(9)
F(1)	F(2)	0.8400(2)	F(1)	F(6)	1.58
F(1)	C(84)	1.3342(3)	F(2)	F(3)	1.6041(3)
F(2)	C(84)	1.31	F(3)	F(4)	1.08
F(3)	C(84)	1.3303(2)	F(4)	F(5)	1.3047(2)
F(4)	C(84)	1.2990(1)	F(5)	F(6)	0.9260(2)
F(5)	C(84)	1.32	F(6)	C(84)	1.3211(3)
F(7)	F(8)	0.9507(2)	F(7)	F(9)	1.6688(5)
F(7)	F(13)	1.20	F(7)	C(85)	1.3584(2)
F(8)	F(9)	0.7871(2)	F(8)	C(85)	1.32
F(9)	F(10)	1.57	F(9)	C(85)	1.3701(1)
F(10)	F(11)	1.0614(2)	F(10)	C(85)	1.3417(2)
F(11)	F(12)	1.0665(3)	F(11)	F(13)	1.6214(4)
F(11)	C(85)	1.25	F(12)	F(13)	0.8584(1)
F(12)	C(85)	1.3498(2)	F(13)	C(85)	1.2917(4)
F(14)	F(15)	0.9261(1)	F(14)	F(16)	1.7021(3)
F(14)	F(19)	1.65	F(14)	F(20)	1.10
F(14)	C(89)	1.2857(1)	F(15)	F(16)	0.9362(2)
F(15)	C(89)	1.32	F(16)	F(17)	1.45
F(16)	C(89)	1.2864(2)	F(17)	F(18)	0.8750(1)
F(17)	C(89)	1.3040(4)	F(18)	F(19)	1.3996(4)
F(18)	C(89)	1.3325(1)	F(19)	F(20)	0.7262(1)

Table 3. Bond Lengths($\AA$) (continued)

atom	atom	distance	atom	atom	distance
F(19)	C(89)	1.3289(1)	F(20)	C(89)	1.3573(2)
F(21)	F(22)	1.3912(2)	F(21)	F(26)	1.1523(2)
F(21)	F(27)	0.6452(1)	F(21)	C(90)	1.16
F(22)	F(23)	1.20	F(22)	C(90)	1.2977(1)
F(23)	F(24)	1.2281(4)	F(23)	C(90)	1.4496(1)
F(24)	F(25)	0.8946(1)	F(24)	C(90)	1.2368(1)
F(25)	F(26)	1.57	F(25)	C(90)	1.3661(3)
F(26)	F(27)	0.7115(1)	F(26)	C(90)	1.3460(2)
F(27)	C(90)	1.41	O(1)	C(6)	1.39(1)
O(1)	C(8)	1.41(1)	O(2)	C(8)	1.44(1)
O(2)	C(9)	1.41(1)	O(3)	C(11)	1.39(1)
O(3)	C(16)	1.40(1)	O(4)	C(16)	1.41(1)
O(4)	C(17)	1.39(1)	O(5)	C(19)	1.40(1)
O(5)	C(24)	1.44(1)	O(6)	C(24)	1.43(1)
O(6)	C(25)	1.39(1)	O(7)	C(27)	1.41(1)
O(7)	C(32)	1.42(1)	O(8)	C(2)	1.38(1)
O(8)	C(32)	1.42(1)	O(9)	C(81)	1.24(1)
O(10)	C(83)	1.26(1)	O(11)	C(86)	1.25(1)
O(12)	C(88)	1.21(2)	O(13)	C(92)	1.22(2)
O(14)	C(92)	1.29(2)	O(14)	C(93)	1.56(2)
O(15)	C(96)	1.1653(1)	O(16)	C(96)	1.37
O(16)	C(97)	1.0838(1)	O(17)	C(100)	1.48
O(18)	C(100)	1.4817(3)	O(18)	C(101)	1.77
N(1)	C(34)	1.33(1)	N(1)	C(35)	1.32(1)

Table 3. Bond Lengths($\AA$) (continued)

atom	atom	distance	atom	atom	distance
N(2)	C(35)	1.33(1)	N(2)	C(36)	1.34(1)
N(3)	C(38)	1.39(1)	N(3)	C(39)	1.30(2)
N(4)	C(39)	1.33(2)	N(4)	C(40)	1.33(1)
N(5)	C(42)	1.34(1)	N(5)	C(43)	1.36(1)
N(6)	C(43)	1.33(2)	N(6)	C(44)	1.34(1)
N(7)	C(46)	1.34(2)	N(7)	C(47)	1.33(2)
N(8)	C(47)	1.26(2)	N(8)	C(48)	1.36(1)
C(1)	C(2)	1.41(1)	C(1)	C(6)	1.42(2)
C(1)	C(33)	1.47(1)	C(2)	C(3)	1.39(1)
C(3)	C(4)	1.39(1)	C(3)	C(31)	1.51(1)
C(4)	C(5)	1.39(1)	C(4)	H(1)	0.96
C(5)	C(6)	1.41(1)	C(5)	C(7)	1.53(1)
C(7)	C(14)	1.50(1)	C(7)	C(49)	1.55(1)
C(7)	H(2)	0.96	C(8)	H(3)	0.97
C(8)	H(4)	0.98	C(9)	C(10)	1.40(1)
C(9)	C(14)	1.37(1)	C(10)	C(11)	1.40(2)
C(10)	C(37)	1.48(1)	C(11)	C(12)	1.39(1)
C(12)	C(13)	1.38(1)	C(12)	C(15)	1.54(1)
C(13)	C(14)	1.40(1)	C(13)	H(5)	0.97
C(15)	C(22)	1.53(2)	C(15)	C(57)	1.53(2)
C(15)	H(6)	0.99	C(16)	H(7)	0.99
C(16)	H(8)	0.98	C(17)	C(18)	1.39(2)
C(17)	C(22)	1.38(1)	C(18)	C(19)	1.39(1)
C(18)	C(41)	1.51(1)	C(19)	C(20)	1.39(1)

Table 3. Bond Lengths($\AA$) (continued)

atom	atom	distance	atom	atom	distance
C(20)	C(21)	1.38(1)	C(20)	C(23)	1.54(1)
C(21)	C(22)	1.41(1)	C(21)	H(9)	0.97
C(23)	C(30)	1.51(1)	C(23)	C(65)	1.54(1)
C(23)	H(10)	0.97	C(24)	H(11)	0.95
C(24)	H(12)	0.95	C(25)	C(26)	1.40(1)
C(25)	C(30)	1.39(1)	C(26)	C(27)	1.40(1)
C(26)	C(45)	1.49(1)	C(27)	C(28)	1.40(1)
C(28)	C(29)	1.41(1)	C(28)	C(31)	1.53(1)
C(29)	C(30)	1.40(1)	C(29)	H(13)	0.95
C(31)	C(73)	1.54(1)	C(31)	H(14)	0.99
C(32)	H(15)	0.99	C(32)	H(16)	0.97
C(33)	C(34)	1.38(2)	C(33)	C(36)	1.38(2)
C(34)	H(17)	1.00	C(35)	H(18)	1.02
C(36)	H(19)	1.01	C(37)	C(38)	1.36(1)
C(37)	C(40)	1.38(1)	C(38)	H(20)	0.99
C(39)	H(21)	0.99	C(40)	H(22)	1.00
C(41)	C(42)	1.37(2)	C(41)	C(44)	1.40(2)
C(42)	H(23)	0.99	C(43)	H(24)	0.99
C(44)	H(25)	1.00	C(45)	C(46)	1.37(2)
C(45)	C(48)	1.34(2)	C(46)	H(26)	1.01
C(47)	H(27)	1.01	C(48)	H(28)	0.98
C(49)	C(50)	1.54(2)	C(49)	H(29)	0.98
C(49)	H(30)	0.97	C(50)	C(51)	1.50(2)
C(50)	H(31)	0.98	C(50)	H(32)	0.97

Table 3. Bond Lengths($\AA$) (continued)

atom	atom	distance	atom	atom	distance
C(51)	C(52)	1.39(2)	C(51)	C(56)	1.36(2)
C(52)	C(53)	1.39(2)	C(52)	H(33)	1.01
C(53)	C(54)	1.40(2)	C(53)	H(34)	0.99
C(54)	C(55)	1.35(2)	C(54)	H(35)	1.01
C(55)	C(56)	1.41(2)	C(55)	H(36)	1.01
C(56)	H(37)	1.03	C(57)	C(58)	1.53(2)
C(57)	H(38)	0.95	C(57)	H(39)	1.01
C(58)	C(59)	1.51(2)	C(58)	H(40)	0.93
C(58)	H(41)	1.01	C(59)	C(60)	1.39(2)
C(59)	C(64)	1.43(2)	C(60)	C(61)	1.39(2)
C(60)	H(42)	0.96	C(61)	C(62)	1.39(2)
C(61)	H(43)	1.03	C(62)	C(63)	1.39(2)
C(62)	H(44)	0.98	C(63)	C(64)	1.38(2)
C(63)	H(45)	1.02	C(64)	H(46)	1.05
C(65)	C(66)	1.52(2)	C(65)	H(47)	0.96
C(65)	H(48)	0.99	C(66)	C(67)	1.49(2)
C(66)	H(49)	0.97	C(66)	H(50)	0.94
C(67)	C(68)	1.38(2)	C(67)	C(72)	1.38(2)
C(68)	C(69)	1.39(2)	C(68)	H(51)	0.98
C(69)	C(70)	1.37(2)	C(69)	H(52)	0.99
C(70)	C(71)	1.37(2)	C(70)	H(53)	1.02
C(71)	C(72)	1.39(2)	C(71)	H(54)	0.99
C(72)	H(55)	0.99	C(73)	C(74)	1.52(1)
C(73)	H(56)	0.97	C(73)	H(57)	1.00

Table 3. Bond Lengths($\AA$) (continued)

atom	atom	distance	atom	atom	distance
C(74)	C(75)	1.53(2)	C(74)	H(58)	0.96
C(74)	H(59)	0.94	C(75)	C(76)	1.38(2)
C(75)	C(80)	1.41(2)	C(76)	C(77)	1.36(2)
C(76)	H(60)	0.98	C(77)	C(78)	1.39(2)
C(77)	H(61)	0.98	C(78)	C(79)	1.36(2)
C(78)	H(62)	0.99	C(79)	C(80)	1.36(2)
C(79)	H(63)	0.98	C(80)	H(64)	0.99
C(81)	C(82)	1.39(2)	C(81)	C(84)	1.55(1)
C(82)	C(83)	1.39(2)	C(82)	H(65)	1.01
C(83)	C(85)	1.53(1)	C(86)	C(87)	1.43(2)
C(86)	C(89)	1.54(1)	C(87)	C(88)	1.40(2)
C(87)	H(66)	1.06	C(88)	C(90)	1.51(1)
C(91)	C(92)	1.49(2)	C(93)	C(94)	1.36(3)
C(95)	C(96)	1.5124(2)	C(97)	C(98)	1.6034(1)
C(99)	C(100)	1.2735(2)	C(101)	C(102)	1.5106(1)

Symmetry operations

(1) X-1,Y,Z-1

Table 4. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
O(9)	Mn(1)	O(10)	84.8(3)	O(9)	Mn(1)	O(11)	101.2(3)
O(9)	Mn(1)	O(12)	174.3(3)	O(9)	Mn(1)	N(2)$^{1)}$	91.7(3)
O(9)	Mn(1)	N(5)	93.2(3)	O(10)	Mn(1)	O(11)	173.4(3)
O(10)	Mn(1)	O(12)	89.9(3)	O(10)	Mn(1)	N(2)$^{1)}$	88.5(3)
O(10)	Mn(1)	N(5)	88.4(3)	O(11)	Mn(1)	O(12)	84.0(3)
O(11)	Mn(1)	N(2)$^{1)}$	88.6(3)	O(11)	Mn(1)	N(5)	94.0(3)
O(12)	Mn(1)	N(2)$^{1)}$	86.2(3)	O(12)	Mn(1)	N(5)	88.6(3)
N(2)$^{1)}$	Mn(1)	N(5)	173.9(4)	F(2)	F(1)	F(6)	120.808(8)
F(2)	F(1)	C(84)	70.12(2)	F(6)	F(1)	C(84)	53.231(8)
F(1)	F(2)	F(3)	122.04(1)	F(1)	F(2)	C(84)	72.89(1)
F(3)	F(2)	C(84)	53.132(2)	F(2)	F(3)	F(4)	106.73(1)
F(2)	F(3)	C(84)	52.139(10)	F(4)	F(3)	C(84)	64.262(2)
F(3)	F(4)	F(5)	126.614(1)	F(3)	F(4)	C(84)	67.294(7)
F(5)	F(4)	C(84)	61.086(7)	F(4)	F(5)	F(6)	126.31(1)
F(4)	F(5)	C(84)	59.244(2)	F(6)	F(5)	C(84)	69.38(1)
F(1)	F(6)	F(5)	113.828(4)	F(1)	F(6)	C(84)	54.001(9)
F(5)	F(6)	C(84)	69.62(1)	F(8)	F(7)	F(9)	14.710(4)
F(8)	F(7)	F(13)	121.090(2)	F(8)	F(7)	C(85)	67.32(2)
F(9)	F(7)	F(13)	107.843(1)	F(9)	F(7)	C(85)	52.61(1)
F(13)	F(7)	C(85)	60.30(1)	F(7)	F(8)	F(9)	147.430(9)
F(7)	F(8)	C(85)	71.188(9)	F(9)	F(8)	C(85)	76.2468(3)
F(7)	F(9)	F(8)	17.860(6)	F(7)	F(9)	F(10)	99.123(6)
F(7)	F(9)	C(85)	51.977(4)	F(8)	F(9)	F(10)	114.965(1)
F(8)	F(9)	C(85)	69.834(9)	F(10)	F(9)	C(85)	53.770(9)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
F(9)	F(10)	F(11)	107.96(1)	F(9)	F(10)	C(85)	55.4575(7)
F(11)	F(10)	C(85)	61.17(1)	F(10)	F(11)	F(12)	141.444(9)
F(10)	F(11)	F(13)	118.38(2)	F(10)	F(11)	C(85)	70.577(8)
F(12)	F(11)	F(13)	28.837(7)	F(12)	F(11)	C(85)	70.922(2)
F(13)	F(11)	C(85)	51.537(7)	F(11)	F(12)	F(13)	114.344(9)
F(11)	F(12)	C(85)	60.77(1)	F(13)	F(12)	C(85)	67.40(2)
F(7)	F(13)	F(11)	105.473(10)	F(7)	F(13)	F(12)	139.79(1)
F(7)	F(13)	C(85)	66.0003(3)	F(11)	F(13)	F(12)	36.818(2)
F(11)	F(13)	C(85)	49.08(1)	F(12)	F(13)	C(85)	74.75(1)
F(15)	F(14)	F(16)	24.084(4)	F(15)	F(14)	F(19)	120.271(6)
F(15)	F(14)	F(20)	139.6167(7)	F(15)	F(14)	C(89)	71.270(8)
F(16)	F(14)	F(19)	96.190(3)	F(16)	F(14)	F(20)	115.679(3)
F(16)	F(14)	C(89)	48.583(4)	F(19)	F(14)	F(20)	20.396(6)
F(19)	F(14)	C(89)	52.167(2)	F(20)	F(14)	C(89)	68.924(7)
F(14)	F(15)	F(16)	132.108(9)	F(14)	F(15)	C(89)	67.142(3)
F(16)	F(15)	C(89)	66.973(6)	F(14)	F(16)	F(15)	23.808(5)
F(14)	F(16)	F(17)	91.666(9)	F(14)	F(16)	C(89)	48.549(8)
F(15)	F(16)	F(17)	114.230(4)	F(15)	F(16)	C(89)	70.97(1)
F(17)	F(16)	C(89)	56.56(1)	F(16)	F(17)	F(18)	127.40(1)
F(16)	F(17)	C(89)	55.4088(4)	F(18)	F(17)	C(89)	72.39(1)
F(17)	F(18)	F(19)	119.705(10)	F(17)	F(18)	C(89)	68.87(2)
F(19)	F(18)	C(89)	58.146(9)	F(14)	F(19)	F(18)	99.163(1)
F(14)	F(19)	F(20)	31.769(7)	F(14)	F(19)	C(89)	49.831(3)
F(18)	F(19)	F(20)	130.799(6)	F(18)	F(19)	C(89)	58.396(4)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
F(20)	F(19)	C(89)	76.484(10)	F(14)	F(20)	F(19)	127.84(1)
F(14)	F(20)	C(89)	62.116(3)	F(19)	F(20)	C(89)	72.167(9)
F(22)	F(21)	F(26)	129.938(8)	F(22)	F(21)	F(27)	159.002(2)
F(22)	F(21)	C(90)	60.370(2)	F(26)	F(21)	F(27)	33.641(4)
F(26)	F(21)	C(90)	71.248(6)	F(27)	F(21)	C(90)	99.2784(9)
F(21)	F(22)	F(23)	119.297(7)	F(21)	F(22)	C(90)	50.904(6)
F(23)	F(22)	C(90)	70.7025(3)	F(22)	F(23)	F(24)	97.268(2)
F(22)	F(23)	C(90)	57.662(4)	F(24)	F(23)	C(90)	54.256(4)
F(23)	F(24)	F(25)	149.177(5)	F(23)	F(24)	C(90)	72.04(1)
F(25)	F(24)	C(90)	77.91(2)	F(24)	F(25)	F(26)	111.586(8)
F(24)	F(25)	C(90)	62.28(1)	F(26)	F(25)	C(90)	53.965(5)
F(21)	F(26)	F(25)	98.290(3)	F(21)	F(26)	F(27)	30.157(5)
F(21)	F(26)	C(90)	54.595(10)	F(25)	F(26)	F(27)	128.445(2)
F(25)	F(26)	C(90)	55.16(1)	F(27)	F(26)	C(90)	80.43(1)
F(21)	F(27)	F(26)	116.202(9)	F(21)	F(27)	C(90)	53.960(3)
F(26)	F(27)	C(90)	69.82(1)	C(6)	O(1)	C(8)	115.8(8)
C(8)	O(2)	C(9)	116.1(8)	C(11)	O(3)	C(16)	117.4(8)
C(16)	O(4)	C(17)	117.1(8)	C(19)	O(5)	C(24)	117.7(8)
C(24)	O(6)	C(25)	116.4(8)	C(27)	O(7)	C(32)	117.4(8)
C(2)	O(8)	C(32)	116.2(8)	Mn(1)	O(9)	C(81)	126.5(9)
Mn(1)	O(10)	C(83)	128.2(9)	Mn(1)	O(11)	C(86)	127.3(8)
Mn(1)	O(12)	C(88)	125.4(9)	C(92)	O(14)	C(93)	117(1)
C(96)	O(16)	C(97)	123.494(2)	C(100)	O(18)	C(101)	118.941(4)
C(34)	N(1)	C(35)	116(1)	Mn(1)[2)]	N(2)	C(35)	125.4(8)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
Mn(1)[2)]	N(2)	C(36)	118.8(8)	C(35)	N(2)	C(36)	115.8(10)
C(38)	N(3)	C(39)	116.4(10)	C(39)	N(4)	C(40)	116(1)
Mn(1)	N(5)	C(42)	123.7(8)	Mn(1)	N(5)	C(43)	121.0(8)
C(42)	N(5)	C(43)	115.4(10)	C(43)	N(6)	C(44)	114(1)
C(46)	N(7)	C(47)	114(1)	C(47)	N(8)	C(48)	113(1)
C(2)	C(1)	C(6)	116(1)	C(2)	C(1)	C(33)	120.8(10)
C(6)	C(1)	C(33)	122(1)	O(8)	C(2)	C(1)	116.9(10)
O(8)	C(2)	C(3)	120.2(10)	C(1)	C(2)	C(3)	122.8(10)
C(2)	C(3)	C(4)	117.3(10)	C(2)	C(3)	C(31)	120.4(10)
C(4)	C(3)	C(31)	122.3(10)	C(3)	C(4)	C(5)	124(1)
C(3)	C(4)	H(1)	119.8	C(5)	C(4)	H(1)	116.0
C(4)	C(5)	C(6)	117(1)	C(4)	C(5)	C(7)	125(1)
C(6)	C(5)	C(7)	117.7(9)	O(1)	C(6)	C(1)	117.3(10)
O(1)	C(6)	C(5)	120.9(10)	C(1)	C(6)	C(5)	121.5(10)
C(5)	C(7)	C(14)	108.7(9)	C(5)	C(7)	C(49)	113.4(9)
C(5)	C(7)	H(2)	107.1	C(14)	C(7)	C(49)	113.7(9)
C(14)	C(7)	H(2)	108.5	C(49)	C(7)	H(2)	105.1
O(1)	C(8)	O(2)	112.6(9)	O(1)	C(8)	H(3)	109.6
O(1)	C(8)	H(4)	108.3	O(2)	C(8)	H(3)	111.5
O(2)	C(8)	H(4)	109.0	H(3)	C(8)	H(4)	105.5
O(2)	C(9)	C(10)	117.0(10)	O(2)	C(9)	C(14)	119.3(10)
C(10)	C(9)	C(14)	123(1)	C(9)	C(10)	C(11)	117(1)
C(9)	C(10)	C(37)	122(1)	C(11)	C(10)	C(37)	120(1)
O(3)	C(11)	C(10)	118.0(10)	O(3)	C(11)	C(12)	120(1)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(10)	C(11)	C(12)	121(1)	C(11)	C(12)	C(13)	117(1)
C(11)	C(12)	C(15)	119.2(10)	C(13)	C(12)	C(15)	123.0(10)
C(12)	C(13)	C(14)	123.2(10)	C(12)	C(13)	H(5)	119.6
C(14)	C(13)	H(5)	117.2	C(7)	C(14)	C(9)	119(1)
C(7)	C(14)	C(13)	123.7(10)	C(9)	C(14)	C(13)	116(1)
C(12)	C(15)	C(22)	107.5(9)	C(12)	C(15)	C(57)	113.5(9)
C(12)	C(15)	H(6)	109.6	C(22)	C(15)	C(57)	114.2(9)
C(22)	C(15)	H(6)	106.7	C(57)	C(15)	H(6)	105.0
O(3)	C(16)	O(4)	112.9(9)	O(3)	C(16)	H(7)	110.4
O(3)	C(16)	H(8)	112.1	O(4)	C(16)	H(7)	108.1
O(4)	C(16)	H(8)	108.7	H(7)	C(16)	H(8)	104.3
O(4)	C(17)	C(18)	118(1)	O(4)	C(17)	C(22)	120(1)
C(18)	C(17)	C(22)	120(1)	C(17)	C(18)	C(19)	119(1)
C(17)	C(18)	C(41)	119.2(9)	C(19)	C(18)	C(41)	121.2(10)
O(5)	C(19)	C(18)	118.1(10)	O(5)	C(19)	C(20)	120.3(10)
C(18)	C(19)	C(20)	121(1)	C(19)	C(20)	C(21)	117.9(10)
C(19)	C(20)	C(23)	120.8(10)	C(21)	C(20)	C(23)	121.3(10)
C(20)	C(21)	C(22)	122.2(10)	C(20)	C(21)	H(9)	118.2
C(22)	C(21)	H(9)	119.5	C(15)	C(22)	C(17)	120(1)
C(15)	C(22)	C(21)	121.1(10)	C(17)	C(22)	C(21)	118(1)
C(20)	C(23)	C(30)	107.7(8)	C(20)	C(23)	C(65)	111.7(9)
C(20)	C(23)	H(10)	107.5	C(30)	C(23)	C(65)	114.9(9)
C(30)	C(23)	H(10)	108.9	C(65)	C(23)	H(10)	105.8
O(5)	C(24)	O(6)	112.4(9)	O(5)	C(24)	H(11)	108.6

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
O(5)	C(24)	H(12)	107.9	O(6)	C(24)	H(11)	109.1
O(6)	C(24)	H(12)	110.0	H(11)	C(24)	H(12)	108.8
O(6)	C(25)	C(26)	117.8(10)	O(6)	C(25)	C(30)	119(1)
C(26)	C(25)	C(30)	122(1)	C(25)	C(26)	C(27)	117(1)
C(25)	C(26)	C(45)	121(1)	C(27)	C(26)	C(45)	121(1)
O(7)	C(27)	C(26)	116.6(9)	O(7)	C(27)	C(28)	120.1(9)
C(26)	C(27)	C(28)	123(1)	C(27)	C(28)	C(29)	116.7(10)
C(27)	C(28)	C(31)	119.6(9)	C(29)	C(28)	C(31)	123.8(10)
C(28)	C(29)	C(30)	122.0(10)	C(28)	C(29)	H(13)	121.5
C(30)	C(29)	H(13)	116.4	C(23)	C(30)	C(25)	118.3(10)
C(23)	C(30)	C(29)	123.2(10)	C(25)	C(30)	C(29)	118(1)
C(3)	C(31)	C(28)	106.9(9)	C(3)	C(31)	C(73)	115.2(9)
C(3)	C(31)	H(14)	108.1	C(28)	C(31)	C(73)	113.6(9)
C(28)	C(31)	H(14)	108.9	C(73)	C(31)	H(14)	104.0
O(7)	C(32)	O(8)	114.5(9)	O(7)	C(32)	H(15)	110.6
O(7)	C(32)	H(16)	111.5	O(8)	C(32)	H(15)	107.2
O(8)	C(32)	H(16)	107.4	H(15)	C(32)	H(16)	105.1
C(1)	C(33)	C(34)	123(1)	C(1)	C(33)	C(36)	120(1)
C(34)	C(33)	C(36)	115(1)	N(1)	C(34)	C(33)	123(1)
N(1)	C(34)	H(17)	120.9	C(33)	C(34)	H(17)	116.0
N(1)	C(35)	N(2)	126(1)	N(1)	C(35)	H(18)	116.3
N(2)	C(35)	H(18)	117.4	N(2)	C(36)	C(33)	122(1)
N(2)	C(36)	H(19)	120.4	C(33)	C(36)	H(19)	116.8
C(10)	C(37)	C(38)	122(1)	C(10)	C(37)	C(40)	122.1(10)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(38)	C(37)	C(40)	115(1)	N(3)	C(38)	C(37)	122(1)
N(3)	C(38)	H(20)	118.7	C(37)	C(38)	H(20)	119.1
N(3)	C(39)	N(4)	125(1)	N(3)	C(39)	H(21)	118.8
N(4)	C(39)	H(21)	115.3	N(4)	C(40)	C(37)	123(1)
N(4)	C(40)	H(22)	116.0	C(37)	C(40)	H(22)	120.4
C(18)	C(41)	C(42)	124(1)	C(18)	C(41)	C(44)	119(1)
C(42)	C(41)	C(44)	116(1)	N(5)	C(42)	C(41)	122(1)
N(5)	C(42)	H(23)	118.1	C(41)	C(42)	H(23)	119.3
N(5)	C(43)	N(6)	127(1)	N(5)	C(43)	H(24)	115.6
N(6)	C(43)	H(24)	116.4	N(6)	C(44)	C(41)	123(1)
N(6)	C(44)	H(25)	119.0	C(41)	C(44)	H(25)	117.2
C(26)	C(45)	C(46)	120(1)	C(26)	C(45)	C(48)	124(1)
C(46)	C(45)	C(48)	114(1)	N(7)	C(46)	C(45)	122(1)
N(7)	C(46)	H(26)	118.5	C(45)	C(46)	H(26)	118.5
N(7)	C(47)	N(8)	128(1)	N(7)	C(47)	H(27)	113.8
N(8)	C(47)	H(27)	117.4	N(8)	C(48)	C(45)	125(1)
N(8)	C(48)	H(28)	118.2	C(45)	C(48)	H(28)	116.0
C(7)	C(49)	C(50)	110.3(9)	C(7)	C(49)	H(29)	111.6
C(7)	C(49)	H(30)	112.7	C(50)	C(49)	H(29)	109.9
C(50)	C(49)	H(30)	106.6	H(29)	C(49)	H(30)	105.5
C(49)	C(50)	C(51)	113.5(9)	C(49)	C(50)	H(31)	104.5
C(49)	C(50)	H(32)	107.8	C(51)	C(50)	H(31)	113.8
C(51)	C(50)	H(32)	111.5	H(31)	C(50)	H(32)	105.1
C(50)	C(51)	C(52)	118(1)	C(50)	C(51)	C(56)	121(1)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(52)	C(51)	C(56)	119(1)	C(51)	C(52)	C(53)	120(1)
C(51)	C(52)	H(33)	118.5	C(53)	C(52)	H(33)	121.1
C(52)	C(53)	C(54)	119(1)	C(52)	C(53)	H(34)	119.2
C(54)	C(53)	H(34)	121.0	C(53)	C(54)	C(55)	119(1)
C(53)	C(54)	H(35)	116.1	C(55)	C(54)	H(35)	123.7
C(54)	C(55)	C(56)	120(1)	C(54)	C(55)	H(36)	119.9
C(56)	C(55)	H(36)	120.0	C(51)	C(56)	C(55)	120(1)
C(51)	C(56)	H(37)	117.3	C(55)	C(56)	H(37)	122.0
C(15)	C(57)	C(58)	113.1(9)	C(15)	C(57)	H(38)	109.1
C(15)	C(57)	H(39)	108.8	C(58)	C(57)	H(38)	110.8
C(58)	C(57)	H(39)	110.0	H(38)	C(57)	H(39)	104.7
C(57)	C(58)	C(59)	112.7(10)	C(57)	C(58)	H(40)	111.3
C(57)	C(58)	H(41)	109.2	C(59)	C(58)	H(40)	109.6
C(59)	C(58)	H(41)	107.9	H(40)	C(58)	H(41)	105.9
C(58)	C(59)	C(60)	120(1)	C(58)	C(59)	C(64)	120(1)
C(60)	C(59)	C(64)	118(1)	C(59)	C(60)	C(61)	121(1)
C(59)	C(60)	H(42)	118.5	C(61)	C(60)	H(42)	119.9
C(60)	C(61)	C(62)	119(1)	C(60)	C(61)	H(43)	121.5
C(62)	C(61)	H(43)	118.5	C(61)	C(62)	C(63)	119(1)
C(61)	C(62)	H(44)	122.0	C(63)	C(62)	H(44)	118.5
C(62)	C(63)	C(64)	121(1)	C(62)	C(63)	H(45)	121.8
C(64)	C(63)	H(45)	116.3	C(59)	C(64)	C(63)	119(1)
C(59)	C(64)	H(46)	118.1	C(63)	C(64)	H(46)	122.7
C(23)	C(65)	C(66)	113.3(9)	C(23)	C(65)	H(47)	110.4

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(23)	C(65)	H(48)	109.7	C(66)	C(65)	H(47)	109.8
C(66)	C(65)	H(48)	107.6	H(47)	C(65)	H(48)	105.7
C(65)	C(66)	C(67)	113.6(10)	C(65)	C(66)	H(49)	105.6
C(65)	C(66)	H(50)	108.3	C(67)	C(66)	H(49)	109.1
C(67)	C(66)	H(50)	111.5	H(49)	C(66)	H(50)	108.3
C(66)	C(67)	C(68)	121(1)	C(66)	C(67)	C(72)	121(1)
C(68)	C(67)	C(72)	116(1)	C(67)	C(68)	C(69)	121(1)
C(67)	C(68)	H(51)	118.3	C(69)	C(68)	H(51)	119.8
C(68)	C(69)	C(70)	120(1)	C(68)	C(69)	H(52)	120.9
C(70)	C(69)	H(52)	118.4	C(69)	C(70)	C(71)	118(1)
C(69)	C(70)	H(53)	123.4	C(71)	C(70)	H(53)	118.3
C(70)	C(71)	C(72)	121(1)	C(70)	C(71)	H(54)	121.2
C(72)	C(71)	H(54)	117.5	C(67)	C(72)	C(71)	120(1)
C(67)	C(72)	H(55)	120.5	C(71)	C(72)	H(55)	118.7
C(31)	C(73)	C(74)	111.8(9)	C(31)	C(73)	H(56)	108.9
C(31)	C(73)	H(57)	109.7	C(74)	C(73)	H(56)	112.6
C(74)	C(73)	H(57)	109.2	H(56)	C(73)	H(57)	104.3
C(73)	C(74)	C(75)	113.0(9)	C(73)	C(74)	H(58)	105.0
C(73)	C(74)	H(59)	109.2	C(75)	C(74)	H(58)	109.2
C(75)	C(74)	H(59)	110.8	H(58)	C(74)	H(59)	109.5
C(74)	C(75)	C(76)	121(1)	C(74)	C(75)	C(80)	120.7(10)
C(76)	C(75)	C(80)	117(1)	C(75)	C(76)	C(77)	121(1)
C(75)	C(76)	H(60)	120.6	C(77)	C(76)	H(60)	117.5
C(76)	C(77)	C(78)	119(1)	C(76)	C(77)	H(61)	121.3

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(78)	C(77)	H(61)	119.2	C(77)	C(78)	C(79)	119(1)
C(77)	C(78)	H(62)	121.8	C(79)	C(78)	H(62)	118.9
C(78)	C(79)	C(80)	122(1)	C(78)	C(79)	H(63)	118.1
C(80)	C(79)	H(63)	119.8	C(75)	C(80)	C(79)	119(1)
C(75)	C(80)	H(64)	119.3	C(79)	C(80)	H(64)	121.2
O(9)	C(81)	C(82)	129(1)	O(9)	C(81)	C(84)	113(1)
C(82)	C(81)	C(84)	116(1)	C(81)	C(82)	C(83)	123(1)
C(81)	C(82)	H(65)	118.1	C(83)	C(82)	H(65)	117.9
O(10)	C(83)	C(82)	126(1)	O(10)	C(83)	C(85)	115(1)
C(82)	C(83)	C(85)	117(1)	F(1)	C(84)	F(2)	36.993(3)
F(1)	C(84)	F(3)	109.05(1)	F(1)	C(84)	F(4)	130.100(5)
F(1)	C(84)	F(5)	106.22(1)	F(1)	C(84)	F(6)	72.77(2)
F(1)	C(84)	C(81)	114.4(5)	F(2)	C(84)	F(3)	74.73(1)
F(2)	C(84)	F(4)	112.828(4)	F(2)	C(84)	F(5)	130.616(8)
F(2)	C(84)	F(6)	108.03(1)	F(2)	C(84)	C(81)	112.7(5)
F(3)	C(84)	F(4)	48.444(5)	F(3)	C(84)	F(5)	106.938(4)
F(3)	C(84)	F(6)	141.063(6)	F(3)	C(84)	C(81)	106.1(5)
F(4)	C(84)	F(5)	59.670(9)	F(4)	C(84)	F(6)	99.36(1)
F(4)	C(84)	C(81)	114.8(5)	F(5)	C(84)	F(6)	40.999(2)
F(5)	C(84)	C(81)	113.8(5)	F(6)	C(84)	C(81)	108.0(5)
F(7)	C(85)	F(8)	41.492(7)	F(7)	C(85)	F(9)	75.41(2)
F(7)	C(85)	F(10)	131.956(9)	F(7)	C(85)	F(11)	120.188(3)
F(7)	C(85)	F(12)	91.20(2)	F(7)	C(85)	F(13)	53.70(1)
F(7)	C(85)	C(83)	111.8(5)	F(8)	C(85)	F(9)	33.920(10)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
F(8)	C(85)	F(10)	99.334(2)	F(8)	C(85)	F(11)	122.1344(1)
F(8)	C(85)	F(12)	124.602(9)	F(8)	C(85)	F(13)	91.589(5)
F(8)	C(85)	C(83)	114.7(5)	F(9)	C(85)	F(10)	70.772(8)
F(9)	C(85)	F(11)	110.402(3)	F(9)	C(85)	F(12)	143.969(2)
F(9)	C(85)	F(13)	122.478(5)	F(9)	C(85)	C(83)	107.6(5)
F(10)	C(85)	F(11)	48.251(6)	F(10)	C(85)	F(12)	96.54(1)
F(10)	C(85)	F(13)	123.69(1)	F(10)	C(85)	C(83)	110.4(5)
F(11)	C(85)	F(12)	48.307(9)	F(11)	C(85)	F(13)	79.387(6)
F(11)	C(85)	C(83)	121.1(5)	F(12)	C(85)	F(13)	37.845(5)
F(12)	C(85)	C(83)	108.4(5)	F(13)	C(85)	C(83)	114.4(5)
O(11)	C(86)	C(87)	125(1)	O(11)	C(86)	C(89)	115(1)
C(87)	C(86)	C(89)	118(1)	C(86)	C(87)	C(88)	123(1)
C(86)	C(87)	H(66)	113.0	C(88)	C(87)	H(66)	123.6
O(12)	C(88)	C(87)	128(1)	O(12)	C(88)	C(90)	117(1)
C(87)	C(88)	C(90)	114(1)	F(14)	C(89)	F(15)	41.588(5)
F(14)	C(89)	F(16)	82.87(1)	F(14)	C(89)	F(17)	122.209(5)
F(14)	C(89)	F(18)	125.150(4)	F(14)	C(89)	F(19)	78.002(5)
F(14)	C(89)	F(20)	48.960(4)	F(14)	C(89)	C(86)	118.1(5)
F(15)	C(89)	F(16)	42.053(6)	F(15)	C(89)	F(17)	100.767(5)
F(15)	C(89)	F(18)	131.101(7)	F(15)	C(89)	F(19)	116.9395(9)
F(15)	C(89)	F(20)	90.3375(9)	F(15)	C(89)	C(86)	113.7(5)
F(16)	C(89)	F(17)	68.03(1)	F(16)	C(89)	F(18)	106.53(2)
F(16)	C(89)	F(19)	144.667(1)	F(16)	C(89)	F(20)	129.522(7)
F(16)	C(89)	C(86)	106.0(5)	F(17)	C(89)	F(18)	38.746(4)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
F(17)	C(89)	F(19)	97.83(1)	F(17)	C(89)	F(20)	121.16(1)
F(17)	C(89)	C(86)	117.5(5)	F(18)	C(89)	F(19)	63.46(1)
F(18)	C(89)	F(20)	93.12(1)	F(18)	C(89)	C(86)	110.9(5)
F(19)	C(89)	F(20)	31.3487(3)	F(19)	C(89)	C(86)	109.2(5)
F(20)	C(89)	C(86)	109.5(5)	F(21)	C(90)	F(22)	68.727(4)
F(21)	C(90)	F(23)	118.0871(4)	F(21)	C(90)	F(24)	122.287(5)
F(21)	C(90)	F(25)	110.622(9)	F(21)	C(90)	F(26)	54.157(4)
F(21)	C(90)	F(27)	26.761(2)	F(21)	C(90)	C(88)	117.7(6)
F(22)	C(90)	F(23)	51.635(4)	F(22)	C(90)	F(24)	92.125(9)
F(22)	C(90)	F(25)	125.588(8)	F(22)	C(90)	F(26)	121.505(8)
F(22)	C(90)	F(27)	95.376(7)	F(22)	C(90)	C(88)	110.7(7)
F(23)	C(90)	F(24)	53.70(1)	F(23)	C(90)	F(25)	93.30(1)
F(23)	C(90)	F(26)	154.2927(7)	F(23)	C(90)	F(27)	144.232(1)
F(23)	C(90)	C(88)	99.0(6)	F(24)	C(90)	F(25)	39.813(1)
F(24)	C(90)	F(26)	106.89(2)	F(24)	C(90)	F(27)	126.03(1)
F(24)	C(90)	C(88)	120.0(6)	F(25)	C(90)	F(26)	70.88(2)
F(25)	C(90)	F(27)	97.51(1)	F(25)	C(90)	C(88)	115.4(7)
F(26)	C(90)	F(27)	29.744(2)	F(26)	C(90)	C(88)	106.1(6)
F(27)	C(90)	C(88)	106.7(5)	O(13)	C(92)	O(14)	121(1)
O(13)	C(92)	C(91)	121(1)	O(14)	C(92)	C(91)	116(1)
O(14)	C(93)	C(94)	113(2)	O(15)	C(96)	O(16)	120.209(8)
O(15)	C(96)	C(95)	129.177(4)	O(16)	C(96)	C(95)	110.606(3)
O(16)	C(97)	C(98)	127.472(3)	O(17)	C(100)	O(18)	115.530(7)
O(17)	C(100)	C(99)	137.547(7)	O(18)	C(100)	C(99)	106.33(1)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
O(18)	C(101)	C(102)	108.485(1)				

Symmetry operations

(1)	X-1,Y,Z-1	(2)	X+1,Y,Z+1

Table 5. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
Mn(1)	O(9)	C(81)	C(82)	3(2)	Mn(1)	O(9)	C(81)	C(84)	-175.2(5)
Mn(1)	O(10)	C(83)	C(82)	6(2)	Mn(1)	O(10)	C(83)	C(85)	-179.7(5)
Mn(1)	O(11)	C(86)	C(87)	14(1)	Mn(1)	O(11)	C(86)	C(89)	-164.8(5)
Mn(1)	O(12)	C(88)	C(87)	-21(2)	Mn(1)	O(12)	C(88)	C(90)	158.4(6)
Mn(1)	N(5)	C(42)	C(41)	179.5(9)	Mn(1)	N(5)	C(43)	N(6)	178(1)
F(1)	F(2)	F(3)	F(4)	10.6948(2)	F(1)	F(2)	F(3)	C(84)	-25.407(1)
F(1)	F(2)	C(84)	F(3)	157.634(4)	F(1)	F(2)	C(84)	F(4)	127.062(3)
F(1)	F(2)	C(84)	F(5)	58.21(1)	F(1)	F(2)	C(84)	F(6)	18.251(5)
F(1)	F(2)	C(84)	C(81)	-100.9(6)	F(1)	F(6)	F(5)	F(4)	14.498(1)
F(1)	F(6)	F(5)	C(84)	31.8414(8)	F(1)	F(6)	C(84)	F(2)	-11.379(1)
F(1)	F(6)	C(84)	F(3)	-99.2049(7)	F(1)	F(6)	C(84)	F(4)	-129.226(3)
F(1)	F(6)	C(84)	F(5)	-143.379(3)	F(1)	F(6)	C(84)	C(81)	110.7(5)
F(1)	C(84)	F(2)	F(3)	-157.634(4)	F(1)	C(84)	F(3)	F(2)	14.0189(4)
F(1)	C(84)	F(3)	F(4)	-127.193(4)	F(1)	C(84)	F(4)	F(3)	79.85(1)
F(1)	C(84)	F(4)	F(5)	-86.01(1)	F(1)	C(84)	F(5)	F(4)	127.37(1)
F(1)	C(84)	F(5)	F(6)	-36.396(10)	F(1)	C(84)	F(6)	F(5)	143.379(3)
F(1)	C(84)	C(81)	O(9)	158.5(9)	F(1)	C(84)	C(81)	C(82)	-20(1)
F(2)	F(1)	F(6)	F(5)	-17.721(3)	F(2)	F(1)	F(6)	C(84)	19.961(6)
F(2)	F(1)	C(84)	F(3)	-22.8529(9)	F(2)	F(1)	C(84)	F(4)	-74.049(3)
F(2)	F(1)	C(84)	F(5)	-137.781(4)	F(2)	F(1)	C(84)	F(6)	-161.833(2)
F(2)	F(1)	C(84)	C(81)	95.8(5)	F(2)	F(3)	F(4)	F(5)	-15.647(3)
F(2)	F(3)	F(4)	C(84)	-31.093(3)	F(2)	F(3)	C(84)	F(4)	141.212(4)
F(2)	F(3)	C(84)	F(5)	128.482(7)	F(2)	F(3)	C(84)	F(6)	99.934(10)
F(2)	F(3)	C(84)	C(81)	-109.7(5)	F(2)	C(84)	F(1)	F(6)	161.833(2)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
F(2)	C(84)	F(3)	F(4)	-141.212(4)	F(2)	C(84)	F(4)	F(3)	40.972(9)
F(2)	C(84)	F(4)	F(5)	-124.892(10)	F(2)	C(84)	F(5)	F(4)	95.19(2)
F(2)	C(84)	F(5)	F(6)	-68.58(1)	F(2)	C(84)	F(6)	F(5)	132.000(4)
F(2)	C(84)	C(81)	O(9)	-161.1(9)	F(2)	C(84)	C(81)	C(82)	20(1)
F(3)	F(2)	F(1)	F(6)	4.1415(1)	F(3)	F(2)	F(1)	C(84)	21.048(1)
F(3)	F(2)	C(84)	F(4)	-30.572(2)	F(3)	F(2)	C(84)	F(5)	-99.42(2)
F(3)	F(2)	C(84)	F(6)	-139.383(9)	F(3)	F(2)	C(84)	C(81)	101.4(6)
F(3)	F(4)	F(5)	F(6)	2.6436(2)	F(3)	F(4)	F(5)	C(84)	-16.301(2)
F(3)	F(4)	C(84)	F(5)	165.8639(8)	F(3)	F(4)	C(84)	F(6)	155.1533(3)
F(3)	F(4)	C(84)	C(81)	-90.0(5)	F(3)	C(84)	F(1)	F(6)	138.980(3)
F(3)	C(84)	F(4)	F(5)	-165.8639(8)	F(3)	C(84)	F(5)	F(4)	11.0
F(3)	C(84)	F(5)	F(6)	-152.755(2)	F(3)	C(84)	F(6)	F(5)	44.174(2)
F(3)	C(84)	C(81)	O(9)	-81(1)	F(3)	C(84)	C(81)	C(82)	100(1)
F(4)	F(3)	F(2)	C(84)	36.1020(9)	F(4)	F(3)	C(84)	F(5)	-12.730(2)
F(4)	F(3)	C(84)	F(6)	-41.278(6)	F(4)	F(3)	C(84)	C(81)	109.1(5)
F(4)	F(5)	F(6)	C(84)	-17.3431(3)	F(4)	F(5)	C(84)	F(6)	163.768(2)
F(4)	F(5)	C(84)	C(81)	-105.9(6)	F(4)	C(84)	F(1)	F(6)	87.783(1)
F(4)	C(84)	F(5)	F(6)	-163.768(2)	F(4)	C(84)	F(6)	F(5)	14.2
F(4)	C(84)	C(81)	O(9)	-30(1)	F(4)	C(84)	C(81)	C(82)	151.4(10)
F(5)	F(4)	F(3)	C(84)	15.4466(5)	F(5)	F(4)	C(84)	F(6)	-10.7106(5)
F(5)	F(4)	C(84)	C(81)	104.2(5)	F(5)	F(6)	F(1)	C(84)	-37.682(8)
F(5)	F(6)	C(84)	C(81)	-105.9(5)	F(5)	C(84)	F(1)	F(6)	24.052(2)
F(5)	C(84)	C(81)	O(9)	36(1)	F(5)	C(84)	C(81)	C(82)	-142(1)
F(6)	F(1)	F(2)	C(84)	-16.906(1)	F(6)	F(1)	C(84)	C(81)	-102.4(5)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
F(6)	F(5)	F(4)	C(84)	18.945(2)	F(6)	F(5)	C(84)	C(81)	90.4(6)
F(6)	C(84)	C(81)	O(9)	79(1)	F(6)	C(84)	C(81)	C(82)	-98(1)
F(7)	F(8)	F(9)	F(10)	-29.0080(1)	F(7)	F(8)	F(9)	C(85)	1.1
F(7)	F(8)	C(85)	F(9)	-179.4015(2)	F(7)	F(8)	C(85)	F(10)	-146.807(6)
F(7)	F(8)	C(85)	F(11)	-100.726(2)	F(7)	F(8)	C(85)	F(12)	-42.12(1)
F(7)	F(8)	C(85)	F(13)	-22.272(7)	F(7)	F(8)	C(85)	C(83)	95.6(6)
F(7)	F(9)	F(8)	C(85)	-1.1	F(7)	F(9)	F(10)	F(11)	-6.029(2)
F(7)	F(9)	F(10)	C(85)	26.992(4)	F(7)	F(9)	C(85)	F(8)	0.4097(1)
F(7)	F(9)	C(85)	F(10)	-145.330(5)	F(7)	F(9)	C(85)	F(11)	-117.230(2)
F(7)	F(9)	C(85)	F(12)	-71.266(9)	F(7)	F(9)	C(85)	F(13)	-27.011(7)
F(7)	F(9)	C(85)	C(83)	108.6(6)	F(7)	F(13)	F(11)	F(10)	-12.7589(5)
F(7)	F(13)	F(11)	F(12)	-162.2668(2)	F(7)	F(13)	F(11)	C(85)	-37.009(3)
F(7)	F(13)	F(12)	F(11)	27.045(5)	F(7)	F(13)	F(12)	C(85)	-12.709(3)
F(7)	F(13)	C(85)	F(8)	18.1541(2)	F(7)	F(13)	C(85)	F(9)	33.0512(5)
F(7)	F(13)	C(85)	F(10)	120.482(1)	F(7)	F(13)	C(85)	F(11)	140.5777(7)
F(7)	F(13)	C(85)	F(12)	171.1	F(7)	F(13)	C(85)	C(83)	-99.9(6)
F(7)	C(85)	F(8)	F(9)	179.4015(2)	F(7)	C(85)	F(9)	F(8)	-0.4097(1)
F(7)	C(85)	F(9)	F(10)	145.330(5)	F(7)	C(85)	F(10)	F(9)	-47.755(6)
F(7)	C(85)	F(10)	F(11)	95.966(8)	F(7)	C(85)	F(11)	F(10)	-121.17(2)
F(7)	C(85)	F(11)	F(12)	60.93(2)	F(7)	C(85)	F(11)	F(13)	36.303(9)
F(7)	C(85)	F(12)	F(11)	-130.916(8)	F(7)	C(85)	F(12)	F(13)	7.199(1)
F(7)	C(85)	F(13)	F(11)	-140.5777(7)	F(7)	C(85)	F(13)	F(12)	-171.1
F(7)	C(85)	C(83)	O(10)	-164.9(9)	F(7)	C(85)	C(83)	C(82)	9(1)
F(8)	F(7)	F(9)	F(10)	153.5603(3)	F(8)	F(7)	F(9)	C(85)	-178.7

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
F(8)	F(7)	F(13)	F(11)	-0.5738(1)	F(8)	F(7)	F(13)	F(12)	-16.997(5)
F(8)	F(7)	F(13)	C(85)	-30.432(9)	F(8)	F(7)	C(85)	F(9)	0.3
F(8)	F(7)	C(85)	F(10)	46.587(2)	F(8)	F(7)	C(85)	F(11)	105.730(5)
F(8)	F(7)	C(85)	F(12)	146.484(4)	F(8)	F(7)	C(85)	F(13)	151.958(4)
F(8)	F(7)	C(85)	C(83)	-103.1(5)	F(8)	F(9)	F(7)	F(13)	-155.5419(3)
F(8)	F(9)	F(7)	C(85)	178.7	F(8)	F(9)	F(10)	F(11)	2.6344(8)
F(8)	F(9)	F(10)	C(85)	35.655(7)	F(8)	F(9)	C(85)	F(10)	-145.740(5)
F(8)	F(9)	C(85)	F(11)	-117.639(1)	F(8)	F(9)	C(85)	F(12)	-71.675(9)
F(8)	F(9)	C(85)	F(13)	-27.421(7)	F(8)	F(9)	C(85)	C(83)	108.2(6)
F(8)	C(85)	F(7)	F(9)	-0.3	F(8)	C(85)	F(7)	F(13)	-151.958(4)
F(8)	C(85)	F(9)	F(10)	145.740(5)	F(8)	C(85)	F(10)	F(9)	-18.564(3)
F(8)	C(85)	F(10)	F(11)	125.157(4)	F(8)	C(85)	F(11)	F(10)	-72.309(8)
F(8)	C(85)	F(11)	F(12)	109.789(9)	F(8)	C(85)	F(11)	F(13)	85.160(2)
F(8)	C(85)	F(12)	F(11)	-104.53(1)	F(8)	C(85)	F(12)	F(13)	33.586(4)
F(8)	C(85)	F(13)	F(11)	-122.4236(5)	F(8)	C(85)	F(13)	F(12)	-152.9019(1)
F(8)	C(85)	C(83)	O(10)	149.9(8)	F(8)	C(85)	C(83)	C(82)	-35(1)
F(9)	F(7)	F(8)	C(85)	1.1	F(9)	F(7)	F(13)	F(11)	6.478(2)
F(9)	F(7)	F(13)	F(12)	-9.946(3)	F(9)	F(7)	F(13)	C(85)	-23.380(7)
F(9)	F(7)	C(85)	F(10)	46.242(2)	F(9)	F(7)	C(85)	F(11)	105.385(5)
F(9)	F(7)	C(85)	F(12)	146.139(4)	F(9)	F(7)	C(85)	F(13)	151.613(4)
F(9)	F(7)	C(85)	C(83)	-103.4(5)	F(9)	F(8)	F(7)	F(13)	27.4013(5)
F(9)	F(8)	F(7)	C(85)	-1.1	F(9)	F(8)	C(85)	F(10)	32.594(6)
F(9)	F(8)	C(85)	F(11)	78.675(2)	F(9)	F(8)	C(85)	F(12)	137.28(1)
F(9)	F(8)	C(85)	F(13)	157.130(7)	F(9)	F(8)	C(85)	C(83)	-85.0(6)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
F(9)	F(10)	F(11)	F(12)	34.004(2)	F(9)	F(10)	F(11)	F(13)	10.8833(8)
F(9)	F(10)	F(11)	C(85)	30.822(2)	F(9)	F(10)	C(85)	F(11)	-143.720(2)
F(9)	F(10)	C(85)	F(12)	-145.297(2)	F(9)	F(10)	C(85)	F(13)	-116.806(1)
F(9)	F(10)	C(85)	C(83)	102.2(5)	F(9)	C(85)	F(7)	F(13)	-151.613(4)
F(9)	C(85)	F(10)	F(11)	143.720(2)	F(9)	C(85)	F(11)	F(10)	-36.592(1)
F(9)	C(85)	F(11)	F(12)	145.506(1)	F(9)	C(85)	F(11)	F(13)	120.877(8)
F(9)	C(85)	F(12)	F(11)	-64.471(6)	F(9)	C(85)	F(12)	F(13)	73.6443(9)
F(9)	C(85)	F(13)	F(11)	-107.5265(2)	F(9)	C(85)	F(13)	F(12)	-138.0048(4)
F(9)	C(85)	C(83)	O(10)	114.2(10)	F(9)	C(85)	C(83)	C(82)	-71(1)
F(10)	F(9)	F(7)	F(13)	-2.0	F(10)	F(9)	F(7)	C(85)	-27.6937(3)
F(10)	F(9)	F(8)	C(85)	-30.0604(1)	F(10)	F(9)	C(85)	F(11)	28.100(3)
F(10)	F(9)	C(85)	F(12)	74.06(1)	F(10)	F(9)	C(85)	F(13)	118.32(1)
F(10)	F(9)	C(85)	C(83)	-106.0(6)	F(10)	F(11)	F(12)	F(13)	-45.750(3)
F(10)	F(11)	F(12)	C(85)	-3.1753(1)	F(10)	F(11)	F(13)	F(12)	149.5079(3)
F(10)	F(11)	F(13)	C(85)	24.251(2)	F(10)	F(11)	C(85)	F(12)	177.9021(4)
F(10)	F(11)	C(85)	F(13)	-157.469(6)	F(10)	F(11)	C(85)	C(83)	90.4(6)
F(10)	C(85)	F(7)	F(13)	-105.371(5)	F(10)	C(85)	F(11)	F(12)	-177.9021(4)
F(10)	C(85)	F(11)	F(13)	157.469(6)	F(10)	C(85)	F(12)	F(11)	1.5753(1)
F(10)	C(85)	F(12)	F(13)	139.690(7)	F(10)	C(85)	F(13)	F(11)	-20.0958(6)
F(10)	C(85)	F(13)	F(12)	-50.574(1)	F(10)	C(85)	C(83)	O(10)	38(1)
F(10)	C(85)	C(83)	C(82)	-146(1)	F(11)	F(10)	F(9)	C(85)	-33.021(6)
F(11)	F(10)	C(85)	F(12)	-1.5766(1)	F(11)	F(10)	C(85)	F(13)	26.914(3)
F(11)	F(10)	C(85)	C(83)	-114.0(5)	F(11)	F(12)	F(13)	C(85)	39.754(8)
F(11)	F(12)	C(85)	F(13)	-138.115(7)	F(11)	F(12)	C(85)	C(83)	115.6(6)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
F(11)	F(13)	F(7)	C(85)	29.858(9)	F(11)	F(13)	F(12)	C(85)	-39.754(8)
F(11)	F(13)	C(85)	F(12)	30.4783(6)	F(11)	F(13)	C(85)	C(83)	119.5(6)
F(11)	C(85)	F(7)	F(13)	-46.228(2)	F(11)	C(85)	F(12)	F(13)	138.115(7)
F(11)	C(85)	F(13)	F(12)	-30.4783(6)	F(11)	C(85)	C(83)	O(10)	-14(1)
F(11)	C(85)	C(83)	C(82)	160.4(9)	F(12)	F(11)	F(10)	C(85)	3.2
F(12)	F(11)	F(13)	C(85)	-125.257(2)	F(12)	F(11)	C(85)	F(13)	24.629(7)
F(12)	F(11)	C(85)	C(83)	-87.5(6)	F(12)	F(13)	F(7)	C(85)	13.435(4)
F(12)	F(13)	F(11)	C(85)	125.257(2)	F(12)	F(13)	C(85)	C(83)	89.0(6)
F(12)	C(85)	F(7)	F(13)	-5.4746(6)	F(12)	C(85)	F(11)	F(13)	-24.629(7)
F(12)	C(85)	C(83)	O(10)	-65(1)	F(12)	C(85)	C(83)	C(82)	108(1)
F(13)	F(7)	F(8)	C(85)	28.4812(5)	F(13)	F(7)	F(9)	C(85)	25.7121(3)
F(13)	F(7)	C(85)	C(83)	104.9(5)	F(13)	F(11)	F(10)	C(85)	-19.9386(7)
F(13)	F(11)	F(12)	C(85)	42.574(3)	F(13)	F(11)	C(85)	C(83)	-112.2(6)
F(13)	F(12)	F(11)	C(85)	-42.574(3)	F(13)	F(12)	C(85)	C(83)	-106.2(6)
F(13)	C(85)	C(83)	O(10)	-106(1)	F(13)	C(85)	C(83)	C(82)	68(1)
F(14)	F(15)	F(16)	F(17)	19.779(2)	F(14)	F(15)	F(16)	C(89)	-17.623(1)
F(14)	F(15)	C(89)	F(16)	165.892(1)	F(14)	F(15)	C(89)	F(17)	127.09(1)
F(14)	F(15)	C(89)	F(18)	99.67(2)	F(14)	F(15)	C(89)	F(19)	22.490(2)
F(14)	F(15)	C(89)	F(20)	5.2353(1)	F(14)	F(15)	C(89)	C(86)	-106.3(5)
F(14)	F(16)	F(15)	C(89)	17.623(1)	F(14)	F(16)	F(17)	F(18)	-27.501(6)
F(14)	F(16)	F(17)	C(89)	-35.627(8)	F(14)	F(16)	C(89)	F(15)	-9.3841(1)
F(14)	F(16)	C(89)	F(17)	129.029(6)	F(14)	F(16)	C(89)	F(18)	124.617(7)
F(14)	F(16)	C(89)	F(19)	57.400(8)	F(14)	F(16)	C(89)	F(20)	16.044(1)
F(14)	F(16)	C(89)	C(86)	-117.2(5)	F(14)	F(19)	F(18)	F(17)	-2.5654(1)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
F(14)	F(19)	F(18)	C(89)	29.956(2)	F(14)	F(19)	F(20)	C(89)	-29.317(2)
F(14)	F(19)	C(89)	F(15)	-15.045(3)	F(14)	F(19)	C(89)	F(16)	-58.72(1)
F(14)	F(19)	C(89)	F(17)	-121.387(4)	F(14)	F(19)	C(89)	F(18)	-139.8257(5)
F(14)	F(19)	C(89)	F(20)	19.716(2)	F(14)	F(19)	C(89)	C(86)	115.8(5)
F(14)	F(20)	F(19)	F(18)	6.1604(9)	F(14)	F(20)	F(19)	C(89)	29.317(2)
F(14)	F(20)	C(89)	F(15)	-4.6058(8)	F(14)	F(20)	C(89)	F(16)	-21.321(4)
F(14)	F(20)	C(89)	F(17)	-107.425(3)	F(14)	F(20)	C(89)	F(18)	-135.806(5)
F(14)	F(20)	C(89)	F(19)	-154.055(4)	F(14)	F(20)	C(89)	C(86)	110.8(5)
F(14)	C(89)	F(15)	F(16)	-165.892(1)	F(14)	C(89)	F(16)	F(15)	9.3841(1)
F(14)	C(89)	F(16)	F(17)	-129.029(6)	F(14)	C(89)	F(17)	F(16)	65.6462(4)
F(14)	C(89)	F(17)	F(18)	-107.5882(5)	F(14)	C(89)	F(18)	F(17)	99.446(2)
F(14)	C(89)	F(18)	F(19)	-50.512(3)	F(14)	C(89)	F(19)	F(18)	139.8257(5)
F(14)	C(89)	F(19)	F(20)	-19.716(2)	F(14)	C(89)	F(20)	F(19)	154.055(4)
F(14)	C(89)	C(86)	O(11)	-1(1)	F(14)	C(89)	C(86)	C(87)	178.7(9)
F(15)	F(14)	F(16)	F(17)	-162.018(2)	F(15)	F(14)	F(16)	C(89)	157.551(3)
F(15)	F(14)	F(19)	F(18)	-11.341(2)	F(15)	F(14)	F(19)	F(20)	163.939(3)
F(15)	F(14)	F(19)	C(89)	22.4761(4)	F(15)	F(14)	F(20)	F(19)	-21.641(3)
F(15)	F(14)	F(20)	C(89)	10.1850(2)	F(15)	F(14)	C(89)	F(16)	-9.5
F(15)	F(14)	C(89)	F(17)	-67.84(1)	F(15)	F(14)	C(89)	F(18)	-114.70(1)
F(15)	F(14)	C(89)	F(19)	-159.596(3)	F(15)	F(14)	C(89)	F(20)	-173.0518(5)
F(15)	F(14)	C(89)	C(86)	94.9(5)	F(15)	F(16)	F(14)	F(19)	179.1384(1)
F(15)	F(16)	F(14)	F(20)	-174.5681(6)	F(15)	F(16)	F(14)	C(89)	-157.551(3)
F(15)	F(16)	F(17)	F(18)	-35.355(6)	F(15)	F(16)	F(17)	C(89)	-43.481(9)
F(15)	F(16)	C(89)	F(17)	138.413(6)	F(15)	F(16)	C(89)	F(18)	134.001(7)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
F(15)	F(16)	C(89)	F(19)	66.784(8)	F(15)	F(16)	C(89)	F(20)	25.428(1)
F(15)	F(16)	C(89)	C(86)	-107.9(5)	F(15)	C(89)	F(14)	F(16)	9.5
F(15)	C(89)	F(14)	F(19)	159.596(3)	F(15)	C(89)	F(14)	F(20)	173.0518(5)
F(15)	C(89)	F(16)	F(17)	-138.413(6)	F(15)	C(89)	F(17)	F(16)	26.9085(4)
F(15)	C(89)	F(17)	F(18)	-146.3259(6)	F(15)	C(89)	F(18)	F(17)	46.290(6)
F(15)	C(89)	F(18)	F(19)	-103.67(1)	F(15)	C(89)	F(19)	F(18)	124.781(4)
F(15)	C(89)	F(19)	F(20)	-34.761(6)	F(15)	C(89)	F(20)	F(19)	149.450(5)
F(15)	C(89)	C(86)	O(11)	44(1)	F(15)	C(89)	C(86)	C(87)	-135(1)
F(16)	F(14)	F(15)	C(89)	-17.600(2)	F(16)	F(14)	F(19)	F(18)	-11.748(2)
F(16)	F(14)	F(19)	F(20)	163.532(3)	F(16)	F(14)	F(19)	C(89)	22.0690(4)
F(16)	F(14)	F(20)	F(19)	-18.223(3)	F(16)	F(14)	F(20)	C(89)	13.6
F(16)	F(14)	C(89)	F(17)	-58.37(1)	F(16)	F(14)	C(89)	F(18)	-105.23(1)
F(16)	F(14)	C(89)	F(19)	-150.126(3)	F(16)	F(14)	C(89)	F(20)	-163.5813(6)
F(16)	F(14)	C(89)	C(86)	104.4(5)	F(16)	F(15)	F(14)	F(19)	-1.0
F(16)	F(15)	F(14)	F(20)	7.5665(5)	F(16)	F(15)	F(14)	C(89)	17.600(2)
F(16)	F(15)	C(89)	F(17)	-38.80(1)	F(16)	F(15)	C(89)	F(18)	-66.22(2)
F(16)	F(15)	C(89)	F(19)	-143.402(1)	F(16)	F(15)	C(89)	F(20)	-160.657(1)
F(16)	F(15)	C(89)	C(86)	87.8(5)	F(16)	F(17)	F(18)	F(19)	22.301(4)
F(16)	F(17)	F(18)	C(89)	-7.012(2)	F(16)	F(17)	C(89)	F(18)	173.2344(1)
F(16)	F(17)	C(89)	F(19)	146.3571(5)	F(16)	F(17)	C(89)	F(20)	123.9154(6)
F(16)	F(17)	C(89)	C(86)	-97.2(5)	F(16)	C(89)	F(14)	F(19)	150.126(3)
F(16)	C(89)	F(14)	F(20)	163.5813(6)	F(16)	C(89)	F(17)	F(18)	-173.2344(1)
F(16)	C(89)	F(18)	F(17)	6.544(1)	F(16)	C(89)	F(18)	F(19)	-143.414(7)
F(16)	C(89)	F(19)	F(18)	81.11(1)	F(16)	C(89)	F(19)	F(20)	-78.43(1)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
F(16)	C(89)	F(20)	F(19)	132.734(8)	F(16)	C(89)	C(86)	O(11)	88.7(10)
F(16)	C(89)	C(86)	C(87)	-90(1)	F(17)	F(16)	F(14)	F(19)	17.120(2)
F(17)	F(16)	F(14)	F(20)	23.414(2)	F(17)	F(16)	F(14)	C(89)	40.430(4)
F(17)	F(16)	F(15)	C(89)	37.402(4)	F(17)	F(16)	C(89)	F(18)	-4.4111(8)
F(17)	F(16)	C(89)	F(19)	-71.629(2)	F(17)	F(16)	C(89)	F(20)	-112.984(5)
F(17)	F(16)	C(89)	C(86)	113.7(5)	F(17)	F(18)	F(19)	F(20)	-5.8461(3)
F(17)	F(18)	F(19)	C(89)	-32.521(2)	F(17)	F(18)	C(89)	F(19)	149.958(5)
F(17)	F(18)	C(89)	F(20)	139.465(6)	F(17)	F(18)	C(89)	C(86)	-108.3(5)
F(17)	C(89)	F(14)	F(19)	91.756(9)	F(17)	C(89)	F(14)	F(20)	105.21(1)
F(17)	C(89)	F(18)	F(19)	-149.958(5)	F(17)	C(89)	F(19)	F(18)	18.438(4)
F(17)	C(89)	F(19)	F(20)	-141.104(6)	F(17)	C(89)	F(20)	F(19)	46.631(1)
F(17)	C(89)	C(86)	O(11)	161.9(8)	F(17)	C(89)	C(86)	C(87)	-17(1)
F(18)	F(17)	F(16)	C(89)	8.126(2)	F(18)	F(17)	C(89)	F(19)	-26.8774(4)
F(18)	F(17)	C(89)	F(20)	-49.3191(4)	F(18)	F(17)	C(89)	C(86)	89.6(5)
F(18)	F(19)	F(14)	F(20)	-175.280(1)	F(18)	F(19)	F(14)	C(89)	-33.817(1)
F(18)	F(19)	F(20)	C(89)	-23.1564(7)	F(18)	F(19)	C(89)	F(20)	159.542(2)
F(18)	F(19)	C(89)	C(86)	-104.3(5)	F(18)	C(89)	F(14)	F(19)	44.90(1)
F(18)	C(89)	F(14)	F(20)	58.35(1)	F(18)	C(89)	F(19)	F(20)	-159.542(2)
F(18)	C(89)	F(20)	F(19)	18.249(1)	F(18)	C(89)	C(86)	O(11)	-156.1(8)
F(18)	C(89)	C(86)	C(87)	24(1)	F(19)	F(14)	F(15)	C(89)	-18.592(2)
F(19)	F(14)	F(16)	C(89)	-23.310(3)	F(19)	F(14)	F(20)	C(89)	31.826(3)
F(19)	F(14)	C(89)	F(20)	-13.456(2)	F(19)	F(14)	C(89)	C(86)	-105.5(5)
F(19)	F(18)	F(17)	C(89)	29.313(5)	F(19)	F(18)	C(89)	F(20)	-10.4926(7)
F(19)	F(18)	C(89)	C(86)	101.7(5)	F(19)	F(20)	F(14)	C(89)	-31.826(3)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
F(19)	F(20)	C(89)	C(86)	-95.2(5)	F(19)	C(89)	F(14)	F(20)	13.456(2)
F(19)	C(89)	C(86)	O(11)	-87(1)	F(19)	C(89)	C(86)	C(87)	92(1)
F(20)	F(14)	F(15)	C(89)	-10.034(1)	F(20)	F(14)	F(16)	C(89)	-17.017(2)
F(20)	F(14)	F(19)	C(89)	-141.463(3)	F(20)	F(14)	C(89)	C(86)	-92.1(5)
F(20)	F(19)	F(14)	C(89)	141.463(3)	F(20)	F(19)	F(18)	C(89)	26.675(2)
F(20)	F(19)	C(89)	C(86)	96.1(5)	F(20)	C(89)	C(86)	O(11)	-54(1)
F(20)	C(89)	C(86)	C(87)	125(1)	F(21)	F(22)	F(23)	F(24)	23.235(4)
F(21)	F(22)	F(23)	C(90)	-15.7116(4)	F(21)	F(22)	C(90)	F(23)	162.284(3)
F(21)	F(22)	C(90)	F(24)	124.00(1)	F(21)	F(22)	C(90)	F(25)	100.73(1)
F(21)	F(22)	C(90)	F(26)	12.669(1)	F(21)	F(22)	C(90)	F(27)	-2.4944(4)
F(21)	F(22)	C(90)	C(88)	-112.7(6)	F(21)	F(26)	F(25)	F(24)	10.4506(8)
F(21)	F(26)	F(25)	C(90)	35.435(6)	F(21)	F(26)	F(27)	C(90)	-28.4229(9)
F(21)	F(26)	C(90)	F(22)	-14.603(1)	F(21)	F(26)	C(90)	F(23)	-80.705(8)
F(21)	F(26)	C(90)	F(24)	-117.991(5)	F(21)	F(26)	C(90)	F(25)	-135.261(2)
F(21)	F(26)	C(90)	F(27)	17.0595(2)	F(21)	F(26)	C(90)	C(88)	112.8(7)
F(21)	F(27)	F(26)	F(25)	-0.7066(1)	F(21)	F(27)	F(26)	C(90)	28.4229(9)
F(21)	F(27)	C(90)	F(22)	5.1676(6)	F(21)	F(27)	C(90)	F(23)	-15.454(3)
F(21)	F(27)	C(90)	F(24)	-91.41(1)	F(21)	F(27)	C(90)	F(25)	-121.844(7)
F(21)	F(27)	C(90)	F(26)	-148.1197(4)	F(21)	F(27)	C(90)	C(88)	118.7(7)
F(21)	C(90)	F(22)	F(23)	-162.284(3)	F(21)	C(90)	F(23)	F(22)	18.748(4)
F(21)	C(90)	F(23)	F(24)	-111.054(2)	F(21)	C(90)	F(24)	F(23)	103.115(9)
F(21)	C(90)	F(24)	F(25)	-83.84(1)	F(21)	C(90)	F(25)	F(24)	116.098(3)
F(21)	C(90)	F(25)	F(26)	-37.564(2)	F(21)	C(90)	F(26)	F(25)	135.261(2)
F(21)	C(90)	F(26)	F(27)	-17.0595(2)	F(21)	C(90)	F(27)	F(26)	148.1197(4)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
F(21)	C(90)	C(88)	O(12)	-41(1)	F(21)	C(90)	C(88)	C(87)	137.6(10)
F(22)	F(21)	F(26)	F(25)	-20.559(3)	F(22)	F(21)	F(26)	F(27)	160.001(3)
F(22)	F(21)	F(26)	C(90)	15.159(2)	F(22)	F(21)	F(27)	F(26)	-47.038(8)
F(22)	F(21)	F(27)	C(90)	-13.499(3)	F(22)	F(21)	C(90)	F(23)	-15.690(2)
F(22)	F(21)	C(90)	F(24)	-78.53(2)	F(22)	F(21)	C(90)	F(25)	-121.38(1)
F(22)	F(21)	C(90)	F(26)	-166.6634(4)	F(22)	F(21)	C(90)	F(27)	174.4779(4)
F(22)	F(21)	C(90)	C(88)	103.0(7)	F(22)	F(23)	F(24)	F(25)	-54.227(1)
F(22)	F(23)	F(24)	C(90)	-40.871(1)	F(22)	F(23)	C(90)	F(24)	129.803(2)
F(22)	F(23)	C(90)	F(25)	134.255(1)	F(22)	F(23)	C(90)	F(26)	83.81(1)
F(22)	F(23)	C(90)	F(27)	26.565(6)	F(22)	F(23)	C(90)	C(88)	-109.4(7)
F(22)	C(90)	F(21)	F(26)	166.6634(4)	F(22)	C(90)	F(21)	F(27)	-174.4779(4)
F(22)	C(90)	F(23)	F(24)	-129.803(2)	F(22)	C(90)	F(24)	F(23)	37.070(4)
F(22)	C(90)	F(24)	F(25)	-149.883(2)	F(22)	C(90)	F(25)	F(24)	38.068(2)
F(22)	C(90)	F(25)	F(26)	-115.5942(7)	F(22)	C(90)	F(26)	F(25)	120.658(1)
F(22)	C(90)	F(26)	F(27)	-31.662(2)	F(22)	C(90)	F(27)	F(26)	153.287(1)
F(22)	C(90)	C(88)	O(12)	34(1)	F(22)	C(90)	C(88)	C(87)	-146(1)
F(23)	F(22)	F(21)	F(26)	2.6761(2)	F(23)	F(22)	F(21)	F(27)	34.597(5)
F(23)	F(22)	F(21)	C(90)	19.228(2)	F(23)	F(22)	C(90)	F(24)	-38.286(7)
F(23)	F(22)	C(90)	F(25)	-61.557(7)	F(23)	F(22)	C(90)	F(26)	-149.615(5)
F(23)	F(22)	C(90)	F(27)	-164.779(3)	F(23)	F(22)	C(90)	C(88)	85.0(6)
F(23)	F(24)	F(25)	F(26)	35.682(2)	F(23)	F(24)	F(25)	C(90)	12.987(1)
F(23)	F(24)	C(90)	F(25)	-173.048(1)	F(23)	F(24)	C(90)	F(26)	160.971(5)
F(23)	F(24)	C(90)	F(27)	135.287(10)	F(23)	F(24)	C(90)	C(88)	-78.4(7)
F(23)	C(90)	F(21)	F(26)	150.973(2)	F(23)	C(90)	F(21)	F(27)	169.832(2)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
F(23)	C(90)	F(24)	F(25)	173.048(1)	F(23)	C(90)	F(25)	F(24)	-5.6
F(23)	C(90)	F(25)	F(26)	-159.2696(7)	F(23)	C(90)	F(26)	F(25)	54.556(6)
F(23)	C(90)	F(26)	F(27)	-97.765(8)	F(23)	C(90)	F(27)	F(26)	132.666(3)
F(23)	C(90)	C(88)	O(12)	86(1)	F(23)	C(90)	C(88)	C(87)	-93(1)
F(24)	F(23)	F(22)	C(90)	38.946(4)	F(24)	F(23)	C(90)	F(25)	4.452(1)
F(24)	F(23)	C(90)	F(26)	-45.99(1)	F(24)	F(23)	C(90)	F(27)	-103.238(4)
F(24)	F(23)	C(90)	C(88)	120.8(7)	F(24)	F(25)	F(26)	F(27)	10.8093(8)
F(24)	F(25)	F(26)	C(90)	-24.984(6)	F(24)	F(25)	C(90)	F(26)	153.6620(8)
F(24)	F(25)	C(90)	F(27)	140.220(2)	F(24)	F(25)	C(90)	C(88)	-107.2(6)
F(24)	C(90)	F(21)	F(26)	88.14(2)	F(24)	C(90)	F(21)	F(27)	107.00(2)
F(24)	C(90)	F(25)	F(26)	-153.6620(8)	F(24)	C(90)	F(26)	F(25)	17.270(3)
F(24)	C(90)	F(26)	F(27)	-135.050(5)	F(24)	C(90)	F(27)	F(26)	56.71(1)
F(24)	C(90)	C(88)	O(12)	139.6(10)	F(24)	C(90)	C(88)	C(87)	-40(1)
F(25)	F(24)	F(23)	C(90)	-13.3554(1)	F(25)	F(24)	C(90)	F(26)	-25.981(6)
F(25)	F(24)	C(90)	F(27)	-51.67(1)	F(25)	F(24)	C(90)	C(88)	94.6(7)
F(25)	F(26)	F(21)	F(27)	179.4407(1)	F(25)	F(26)	F(21)	C(90)	-35.718(4)
F(25)	F(26)	F(27)	C(90)	-29.129(1)	F(25)	F(26)	C(90)	F(27)	152.320(3)
F(25)	F(26)	C(90)	C(88)	-111.9(7)	F(25)	C(90)	F(21)	F(26)	45.28(1)
F(25)	C(90)	F(21)	F(27)	64.14(1)	F(25)	C(90)	F(26)	F(27)	-152.320(3)
F(25)	C(90)	F(27)	F(26)	26.275(6)	F(25)	C(90)	C(88)	O(12)	-175.4(10)
F(25)	C(90)	C(88)	C(87)	4(1)	F(26)	F(21)	F(22)	C(90)	-16.551(2)
F(26)	F(21)	F(27)	C(90)	33.539(6)	F(26)	F(21)	C(90)	F(27)	-18.8588(1)
F(26)	F(21)	C(90)	C(88)	-90.4(7)	F(26)	F(25)	F(24)	C(90)	22.6955(6)
F(26)	F(25)	C(90)	F(27)	-13.4415(8)	F(26)	F(25)	C(90)	C(88)	99.2(6)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
F(26)	F(27)	F(21)	C(90)	-33.539(6)	F(26)	F(27)	C(90)	C(88)	-93.2(7)
F(26)	C(90)	F(21)	F(27)	18.8588(1)	F(26)	C(90)	C(88)	O(12)	-99(1)
F(26)	C(90)	C(88)	C(87)	80(1)	F(27)	F(21)	F(22)	C(90)	15.369(3)
F(27)	F(21)	F(26)	C(90)	-144.841(4)	F(27)	F(21)	C(90)	C(88)	-71.5(7)
F(27)	F(26)	F(21)	C(90)	144.841(4)	F(27)	F(26)	F(25)	C(90)	35.793(6)
F(27)	F(26)	C(90)	C(88)	95.8(7)	F(27)	C(90)	C(88)	O(12)	-68(1)
F(27)	C(90)	C(88)	C(87)	111(1)	O(1)	C(6)	C(1)	C(2)	179.3(9)
O(1)	C(6)	C(1)	C(33)	0(1)	O(1)	C(6)	C(5)	C(4)	-178.4(10)
O(1)	C(6)	C(5)	C(7)	4(1)	O(1)	C(8)	O(2)	C(9)	-94(1)
O(2)	C(8)	O(1)	C(6)	93(1)	O(2)	C(9)	C(10)	C(11)	-176.9(9)
O(2)	C(9)	C(10)	C(37)	-2(1)	O(2)	C(9)	C(14)	C(7)	-3(1)
O(2)	C(9)	C(14)	C(13)	178.8(9)	O(3)	C(11)	C(10)	C(9)	177.2(9)
O(3)	C(11)	C(10)	C(37)	2(1)	O(3)	C(11)	C(12)	C(13)	-177.2(9)
O(3)	C(11)	C(12)	C(15)	6(1)	O(3)	C(16)	O(4)	C(17)	-89(1)
O(4)	C(16)	O(3)	C(11)	92(1)	O(4)	C(17)	C(18)	C(19)	-176.1(10)
O(4)	C(17)	C(18)	C(41)	3(1)	O(4)	C(17)	C(22)	C(15)	-7(1)
O(4)	C(17)	C(22)	C(21)	175.6(9)	O(5)	C(19)	C(18)	C(17)	173.7(10)
O(5)	C(19)	C(18)	C(41)	-6(1)	O(5)	C(19)	C(20)	C(21)	-176.9(9)
O(5)	C(19)	C(20)	C(23)	5(1)	O(5)	C(24)	O(6)	C(25)	-95(1)
O(6)	C(24)	O(5)	C(19)	90(1)	O(6)	C(25)	C(26)	C(27)	178.9(9)
O(6)	C(25)	C(26)	C(45)	-2(1)	O(6)	C(25)	C(30)	C(23)	0(1)
O(6)	C(25)	C(30)	C(29)	179.6(9)	O(7)	C(27)	C(26)	C(25)	178.4(9)
O(7)	C(27)	C(26)	C(45)	0(1)	O(7)	C(27)	C(28)	C(29)	-177.4(9)
O(7)	C(27)	C(28)	C(31)	3(1)	O(7)	C(32)	O(8)	C(2)	-91(1)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
O(8)	C(2)	C(1)	C(6)	-178.5(9)	O(8)	C(2)	C(1)	C(33)	0(1)
O(8)	C(2)	C(3)	C(4)	175.7(10)	O(8)	C(2)	C(3)	C(31)	-5(1)
O(8)	C(32)	O(7)	C(27)	90(1)	O(9)	Mn(1)	O(10)	C(83)	-3(1)
O(9)	Mn(1)	O(11)	C(86)	156(1)	O(9)	Mn(1)	O(12)	C(88)	-133(3)
O(9)	Mn(1)	N(5)	C(42)	-140.9(9)	O(9)	Mn(1)	N(5)	C(43)	39.9(10)
O(9)	C(81)	C(82)	C(83)	-1(2)	O(10)	Mn(1)	O(9)	C(81)	0(1)
O(10)	Mn(1)	O(11)	C(86)	0(3)	O(10)	Mn(1)	O(12)	C(88)	-153(1)
O(10)	Mn(1)	N(5)	C(42)	-56.2(9)	O(10)	Mn(1)	N(5)	C(43)	124.6(10)
O(10)	C(83)	C(82)	C(81)	-3(2)	O(11)	Mn(1)	O(9)	C(81)	-177(1)
O(11)	Mn(1)	O(10)	C(83)	151(2)	O(11)	Mn(1)	O(12)	C(88)	24(1)
O(11)	Mn(1)	N(5)	C(42)	117.5(9)	O(11)	Mn(1)	N(5)	C(43)	-61.6(10)
O(11)	C(86)	C(87)	C(88)	0(2)	O(12)	Mn(1)	O(9)	C(81)	-21(3)
O(12)	Mn(1)	O(10)	C(83)	174(1)	O(12)	Mn(1)	O(11)	C(86)	-21(1)
O(12)	Mn(1)	N(5)	C(42)	33.7(9)	O(12)	Mn(1)	N(5)	C(43)	-145.5(10)
O(12)	C(88)	C(87)	C(86)	3(2)	O(13)	C(92)	O(14)	C(93)	-5(2)
O(15)	C(96)	O(16)	C(97)	-12.5334(9)	O(17)	C(100)	O(18)	C(101)	172.7004(3)
N(1)	C(34)	C(33)	C(1)	178(1)	N(1)	C(34)	C(33)	C(36)	-1(1)
N(1)	C(35)	N(2)	C(36)	0(1)	N(2)	C(35)	N(1)	C(34)	0(1)
N(2)	C(36)	C(33)	C(1)	-179(1)	N(2)	C(36)	C(33)	C(34)	0(1)
N(3)	C(38)	C(37)	C(10)	-179(1)	N(3)	C(38)	C(37)	C(40)	0(1)
N(3)	C(39)	N(4)	C(40)	0(2)	N(4)	C(39)	N(3)	C(38)	-1(2)
N(4)	C(40)	C(37)	C(10)	178(1)	N(4)	C(40)	C(37)	C(38)	0(1)
N(5)	Mn(1)	O(9)	C(81)	87(1)	N(5)	Mn(1)	O(10)	C(83)	-97(1)
N(5)	Mn(1)	O(11)	C(86)	-109(1)	N(5)	Mn(1)	O(12)	C(88)	118(1)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
N(5)	C(42)	C(41)	C(18)	178(1)	N(5)	C(42)	C(41)	C(44)	1(1)
N(5)	C(43)	N(6)	C(44)	1(2)	N(6)	C(43)	N(5)	C(42)	0(1)
N(6)	C(44)	C(41)	C(18)	-176(1)	N(6)	C(44)	C(41)	C(42)	0(1)
N(7)	C(46)	C(45)	C(26)	179(1)	N(7)	C(46)	C(45)	C(48)	0(2)
N(7)	C(47)	N(8)	C(48)	3(2)	N(8)	C(47)	N(7)	C(46)	-4(2)
N(8)	C(48)	C(45)	C(26)	-179(1)	N(8)	C(48)	C(45)	C(46)	0(2)
C(1)	C(2)	O(8)	C(32)	-101(1)	C(1)	C(2)	C(3)	C(4)	0(1)
C(1)	C(2)	C(3)	C(31)	178(1)	C(1)	C(6)	O(1)	C(8)	104(1)
C(1)	C(6)	C(5)	C(4)	-3(1)	C(1)	C(6)	C(5)	C(7)	179.1(10)
C(2)	C(1)	C(6)	C(5)	4(1)	C(2)	C(1)	C(33)	C(34)	122(1)
C(2)	C(1)	C(33)	C(36)	-56(1)	C(2)	C(3)	C(4)	C(5)	0(1)
C(2)	C(3)	C(31)	C(28)	-86(1)	C(2)	C(3)	C(31)	C(73)	146.3(10)
C(3)	C(2)	O(8)	C(32)	82(1)	C(3)	C(2)	C(1)	C(6)	-2(1)
C(3)	C(2)	C(1)	C(33)	175(1)	C(3)	C(4)	C(5)	C(6)	1(1)
C(3)	C(4)	C(5)	C(7)	177(1)	C(3)	C(31)	C(28)	C(27)	86(1)
C(3)	C(31)	C(28)	C(29)	-92(1)	C(3)	C(31)	C(73)	C(74)	-173.0(9)
C(4)	C(3)	C(31)	C(28)	92(1)	C(4)	C(3)	C(31)	C(73)	-34(1)
C(4)	C(5)	C(7)	C(14)	-89(1)	C(4)	C(5)	C(7)	C(49)	38(1)
C(5)	C(4)	C(3)	C(31)	-178(1)	C(5)	C(6)	O(1)	C(8)	-80(1)
C(5)	C(6)	C(1)	C(33)	-173(1)	C(5)	C(7)	C(14)	C(9)	-88(1)
C(5)	C(7)	C(14)	C(13)	89(1)	C(5)	C(7)	C(49)	C(50)	66(1)
C(6)	C(1)	C(33)	C(34)	-59(1)	C(6)	C(1)	C(33)	C(36)	121(1)
C(6)	C(5)	C(7)	C(14)	87(1)	C(6)	C(5)	C(7)	C(49)	-145.2(10)
C(7)	C(14)	C(9)	C(10)	-179.6(10)	C(7)	C(14)	C(13)	C(12)	179.7(10)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(7)	C(49)	C(50)	C(51)	62(1)	C(8)	O(2)	C(9)	C(10)	-102(1)
C(8)	O(2)	C(9)	C(14)	80(1)	C(9)	C(10)	C(11)	C(12)	-1(1)
C(9)	C(10)	C(37)	C(38)	71(1)	C(9)	C(10)	C(37)	C(40)	-106(1)
C(9)	C(14)	C(7)	C(49)	144.0(10)	C(9)	C(14)	C(13)	C(12)	-2(1)
C(10)	C(9)	C(14)	C(13)	2(1)	C(10)	C(11)	O(3)	C(16)	96(1)
C(10)	C(11)	C(12)	C(13)	1(1)	C(10)	C(11)	C(12)	C(15)	-174.4(10)
C(11)	C(10)	C(9)	C(14)	0(1)	C(11)	C(10)	C(37)	C(38)	-113(1)
C(11)	C(10)	C(37)	C(40)	67(1)	C(11)	C(12)	C(13)	C(14)	0(1)
C(11)	C(12)	C(15)	C(22)	83(1)	C(11)	C(12)	C(15)	C(57)	-149.3(10)
C(12)	C(11)	O(3)	C(16)	-85(1)	C(12)	C(11)	C(10)	C(37)	-176.5(10)
C(12)	C(15)	C(22)	C(17)	-83(1)	C(12)	C(15)	C(22)	C(21)	93(1)
C(12)	C(15)	C(57)	C(58)	62(1)	C(13)	C(12)	C(15)	C(22)	-92(1)
C(13)	C(12)	C(15)	C(57)	35(1)	C(13)	C(14)	C(7)	C(49)	-38(1)
C(14)	C(7)	C(49)	C(50)	-168.3(8)	C(14)	C(9)	C(10)	C(37)	174(1)
C(14)	C(13)	C(12)	C(15)	176.4(10)	C(15)	C(22)	C(17)	C(18)	173.1(10)
C(15)	C(22)	C(21)	C(20)	-176(1)	C(15)	C(57)	C(58)	C(59)	-176.3(9)
C(16)	O(4)	C(17)	C(18)	-97(1)	C(16)	O(4)	C(17)	C(22)	82(1)
C(17)	C(18)	C(19)	C(20)	0(1)	C(17)	C(18)	C(41)	C(42)	-56(1)
C(17)	C(18)	C(41)	C(44)	120(1)	C(17)	C(22)	C(15)	C(57)	149(1)
C(17)	C(22)	C(21)	C(20)	0(1)	C(18)	C(17)	C(22)	C(21)	-4(1)
C(18)	C(19)	O(5)	C(24)	107(1)	C(18)	C(19)	C(20)	C(21)	-3(1)
C(18)	C(19)	C(20)	C(23)	178(1)	C(19)	C(18)	C(17)	C(22)	3(1)
C(19)	C(18)	C(41)	C(42)	123(1)	C(19)	C(18)	C(41)	C(44)	-59(1)
C(19)	C(20)	C(21)	C(22)	3(1)	C(19)	C(20)	C(23)	C(30)	85(1)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(19)	C(20)	C(23)	C(65)	-147(1)	C(20)	C(19)	O(5)	C(24)	-78(1)
C(20)	C(19)	C(18)	C(41)	-179(1)	C(20)	C(23)	C(30)	C(25)	-89(1)
C(20)	C(23)	C(30)	C(29)	90(1)	C(20)	C(23)	C(65)	C(66)	61(1)
C(21)	C(20)	C(23)	C(30)	-92(1)	C(21)	C(20)	C(23)	C(65)	34(1)
C(21)	C(22)	C(15)	C(57)	-33(1)	C(22)	C(15)	C(57)	C(58)	-173.6(9)
C(22)	C(17)	C(18)	C(41)	-176.5(10)	C(22)	C(21)	C(20)	C(23)	-179.5(10)
C(23)	C(30)	C(25)	C(26)	178.5(10)	C(23)	C(30)	C(29)	C(28)	-177.6(10)
C(23)	C(65)	C(66)	C(67)	-171.0(10)	C(24)	O(6)	C(25)	C(26)	-96(1)
C(24)	O(6)	C(25)	C(30)	81(1)	C(25)	C(26)	C(27)	C(28)	0(1)
C(25)	C(26)	C(45)	C(46)	-81(1)	C(25)	C(26)	C(45)	C(48)	97(1)
C(25)	C(30)	C(23)	C(65)	144(1)	C(25)	C(30)	C(29)	C(28)	3(1)
C(26)	C(25)	C(30)	C(29)	-2(1)	C(26)	C(27)	O(7)	C(32)	102(1)
C(26)	C(27)	C(28)	C(29)	0(1)	C(26)	C(27)	C(28)	C(31)	-178.0(10)
C(27)	C(26)	C(25)	C(30)	0(1)	C(27)	C(26)	C(45)	C(46)	96(1)
C(27)	C(26)	C(45)	C(48)	-83(1)	C(27)	C(28)	C(29)	C(30)	-2(1)
C(27)	C(28)	C(31)	C(73)	-145.5(10)	C(28)	C(27)	O(7)	C(32)	-79(1)
C(28)	C(27)	C(26)	C(45)	-178.7(10)	C(28)	C(31)	C(73)	C(74)	63(1)
C(29)	C(28)	C(31)	C(73)	35(1)	C(29)	C(30)	C(23)	C(65)	-34(1)
C(30)	C(23)	C(65)	C(66)	-175.0(9)	C(30)	C(25)	C(26)	C(45)	179(1)
C(30)	C(29)	C(28)	C(31)	176.4(10)	C(31)	C(73)	C(74)	C(75)	61(1)
C(33)	C(34)	N(1)	C(35)	1(1)	C(33)	C(36)	N(2)	C(35)	0(1)
C(37)	C(38)	N(3)	C(39)	1(1)	C(37)	C(40)	N(4)	C(39)	1(2)
C(41)	C(42)	N(5)	C(43)	-1(1)	C(41)	C(44)	N(6)	C(43)	-1(1)
C(45)	C(46)	N(7)	C(47)	1(2)	C(45)	C(48)	N(8)	C(47)	-1(2)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(49)	C(50)	C(51)	C(52)	-107(1)	C(49)	C(50)	C(51)	C(56)	71(1)
C(50)	C(51)	C(52)	C(53)	-179(1)	C(50)	C(51)	C(56)	C(55)	178(1)
C(51)	C(52)	C(53)	C(54)	0(2)	C(51)	C(56)	C(55)	C(54)	1(2)
C(52)	C(51)	C(56)	C(55)	-3(1)	C(52)	C(53)	C(54)	C(55)	-1(2)
C(53)	C(52)	C(51)	C(56)	2(1)	C(53)	C(54)	C(55)	C(56)	1(2)
C(57)	C(58)	C(59)	C(60)	118(1)	C(57)	C(58)	C(59)	C(64)	-59(1)
C(58)	C(59)	C(60)	C(61)	-179(1)	C(58)	C(59)	C(64)	C(63)	-179(1)
C(59)	C(60)	C(61)	C(62)	0(2)	C(59)	C(64)	C(63)	C(62)	-2(2)
C(60)	C(59)	C(64)	C(63)	1(1)	C(60)	C(61)	C(62)	C(63)	0(2)
C(61)	C(60)	C(59)	C(64)	0(2)	C(61)	C(62)	C(63)	C(64)	1(2)
C(65)	C(66)	C(67)	C(68)	69(1)	C(65)	C(66)	C(67)	C(72)	-106(1)
C(66)	C(67)	C(68)	C(69)	-178(1)	C(66)	C(67)	C(72)	C(71)	179(1)
C(67)	C(68)	C(69)	C(70)	0(2)	C(67)	C(72)	C(71)	C(70)	-2(2)
C(68)	C(67)	C(72)	C(71)	3(1)	C(68)	C(69)	C(70)	C(71)	1(2)
C(69)	C(68)	C(67)	C(72)	-2(1)	C(69)	C(70)	C(71)	C(72)	0(2)
C(73)	C(74)	C(75)	C(76)	-103(1)	C(73)	C(74)	C(75)	C(80)	76(1)
C(74)	C(75)	C(76)	C(77)	177(1)	C(74)	C(75)	C(80)	C(79)	-179(1)
C(75)	C(76)	C(77)	C(78)	1(1)	C(75)	C(80)	C(79)	C(78)	4(1)
C(76)	C(75)	C(80)	C(79)	0(1)	C(76)	C(77)	C(78)	C(79)	2(1)
C(77)	C(76)	C(75)	C(80)	-2(1)	C(77)	C(78)	C(79)	C(80)	-4(2)
C(81)	C(82)	C(83)	C(85)	-177(1)	C(83)	C(82)	C(81)	C(84)	176(1)
C(86)	C(87)	C(88)	C(90)	-175(1)	C(88)	C(87)	C(86)	C(89)	179(1)
C(91)	C(92)	O(14)	C(93)	175(1)	C(92)	O(14)	C(93)	C(94)	179(2)
C(95)	C(96)	O(16)	C(97)	168.3615(9)	C(96)	O(16)	C(97)	C(98)	175.419(1)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(99)	C(100)	O(18)	C(101)	-14.5529(2)	C(100)	O(18)	C(101)	C(102)	100.94(2)

Table 6. Non-bonded Contacts out to 3.80 $\AA$

atom	atom	distance	atom	atom	distance
Mn(1)	H(21)$^{1)}$	3.71	F(1)	N(6)$^{1)}$	3.39(1)
F(1)	H(24)$^{1)}$	3.52	F(1)	N(3)$^{2)}$	3.63(1)
F(1)	C(43)$^{1)}$	3.70(1)	F(1)	C(39)$^{2)}$	3.74(1)
F(1)	H(21)$^{2)}$	3.75	F(2)	H(21)$^{2)}$	2.98
F(2)	C(39)$^{2)}$	3.08(1)	F(2)	H(24)$^{1)}$	3.11
F(2)	N(3)$^{2)}$	3.18(1)	F(2)	C(43)$^{1)}$	3.40(1)
F(2)	N(6)$^{1)}$	3.40(1)	F(2)	F(20)$^{1)}$	3.538(1)
F(3)	F(20)$^{1)}$	2.5819(6)	F(3)	F(19)$^{1)}$	2.6617(8)
F(3)	H(27)$^{3)}$	2.85	F(3)	H(21)$^{2)}$	3.23
F(3)	F(14)$^{1)}$	3.4927(5)	F(3)	O(11)$^{1)}$	3.493(8)
F(3)	C(86)$^{1)}$	3.59(1)	F(3)	C(89)$^{1)}$	3.5886(8)
F(3)	H(24)$^{1)}$	3.70	F(3)	C(39)$^{2)}$	3.75(1)
F(3)	C(47)$^{3)}$	3.75(1)	F(3)	C(43)$^{1)}$	3.80(1)
F(4)	H(27)$^{3)}$	2.55	F(4)	H(8)$^{1)}$	3.23
F(4)	F(19)$^{1)}$	3.3509(7)	F(4)	C(47)$^{3)}$	3.37(1)
F(4)	F(20)$^{1)}$	3.4482(5)	F(4)	N(7)$^{3)}$	3.52(1)
F(4)	H(7)$^{1)}$	3.73	F(5)	N(3)$^{1)}$	3.24(1)
F(5)	H(20)$^{1)}$	3.37	F(5)	C(38)$^{1)}$	3.49(1)
F(5)	H(27)$^{3)}$	3.52	F(5)	H(7)$^{1)}$	3.71
F(5)	H(8)$^{1)}$	3.74	F(6)	O(18)$^{1)}$	3.1412(2)
F(6)	C(93)$^{1)}$	3.63(3)	F(6)	H(20)$^{1)}$	3.79
F(7)	O(2)$^{2)}$	2.842(7)	F(7)	H(22)$^{2)}$	3.40
F(7)	C(40)$^{2)}$	3.45(1)	F(7)	C(102)$^{1)}$	3.5235(6)
F(7)	C(9)$^{2)}$	3.55(1)	F(7)	C(37)$^{2)}$	3.65(1)

Table 6. Non-bonded Contacts out to 3.80 $\AA$ (continued)

atom	atom	distance	atom	atom	distance
F(8)	H(22)$^{2)}$	2.77	F(8)	C(40)$^{2)}$	3.01(1)
F(8)	O(2)$^{2)}$	3.432(7)	F(8)	N(4)$^{2)}$	3.48(1)
F(8)	C(37)$^{2)}$	3.54(1)	F(9)	H(22)$^{2)}$	2.86
F(9)	C(40)$^{2)}$	3.24(1)	F(9)	N(4)$^{2)}$	3.57(1)
F(10)	H(43)$^{4)}$	2.86	F(10)	H(44)$^{4)}$	3.46
F(10)	C(61)$^{4)}$	3.72(1)	F(10)	C(98)$^{4)}$	3.7940(7)
F(11)	H(43)$^{4)}$	2.50	F(11)	H(44)$^{4)}$	2.88
F(11)	C(61)$^{4)}$	3.21(1)	F(11)	C(62)$^{4)}$	3.36(1)
F(12)	H(44)$^{4)}$	3.10	F(12)	H(43)$^{4)}$	3.17
F(12)	H(36)$^{2)}$	3.55	F(12)	C(62)$^{4)}$	3.63(1)
F(12)	C(101)$^{1)}$	3.6320(5)	F(12)	C(102)$^{1)}$	3.6371(7)
F(12)	C(55)$^{2)}$	3.65(1)	F(12)	C(61)$^{4)}$	3.68(1)
F(12)	H(35)$^{2)}$	3.72	F(12)	C(54)$^{2)}$	3.77(2)
F(13)	C(102)$^{1)}$	3.1803(6)	F(13)	O(2)$^{2)}$	3.422(7)
F(13)	C(101)$^{1)}$	3.5052(3)	F(14)	H(21)$^{1)}$	2.56
F(14)	H(15)$^{3)}$	2.76	F(14)	N(4)$^{1)}$	3.114(10)
F(14)	C(39)$^{1)}$	3.21(1)	F(14)	H(16)$^{3)}$	3.37
F(14)	C(32)$^{3)}$	3.53(1)	F(14)	N(8)$^{3)}$	3.62(1)
F(14)	H(28)$^{3)}$	3.65	F(14)	C(48)$^{3)}$	3.75(2)
F(15)	H(28)$^{3)}$	3.02	F(15)	H(21)$^{1)}$	3.03
F(15)	N(8)$^{3)}$	3.09(1)	F(15)	H(15)$^{3)}$	3.14
F(15)	C(48)$^{3)}$	3.24(1)	F(15)	H(16)$^{3)}$	3.35
F(15)	N(4)$^{1)}$	3.560(10)	F(15)	C(39)$^{1)}$	3.70(1)
F(15)	C(32)$^{3)}$	3.73(1)	F(16)	H(28)$^{3)}$	3.28

Table 6. Non-bonded Contacts out to 3.80 $\AA$ (continued)

atom	atom	distance	atom	atom	distance
F(16)	N(8)$^{3)}$	3.49(1)	F(16)	C(93)$^{3)}$	3.50(3)
F(16)	C(48)$^{3)}$	3.68(1)	F(16)	C(94)$^{3)}$	3.70(3)
F(17)	C(99)$^{3)}$	3.2049(6)	F(17)	N(1)$^{3)}$	3.36(1)
F(17)	O(17)$^{3)}$	3.425(1)	F(17)	C(100)$^{3)}$	3.481(1)
F(17)	C(34)$^{3)}$	3.76(1)	F(18)	H(27)$^{5)}$	3.00
F(18)	N(1)$^{3)}$	3.12(1)	F(18)	C(47)$^{5)}$	3.30(1)
F(18)	C(35)$^{3)}$	3.44(1)	F(18)	H(18)$^{3)}$	3.47
F(18)	C(99)$^{3)}$	3.5307(7)	F(18)	N(8)$^{5)}$	3.58(1)
F(18)	C(34)$^{3)}$	3.76(1)	F(19)	H(27)$^{5)}$	2.68
F(19)	C(47)$^{5)}$	3.36(1)	F(19)	H(21)$^{1)}$	3.45
F(19)	C(35)$^{3)}$	3.45(1)	F(19)	H(18)$^{3)}$	3.50
F(19)	N(1)$^{3)}$	3.57(1)	F(19)	C(81)$^{6)}$	3.70(1)
F(19)	C(84)$^{6)}$	3.738(1)	F(19)	H(15)$^{3)}$	3.75
F(20)	H(21)$^{1)}$	2.80	F(20)	H(15)$^{3)}$	3.23
F(20)	H(27)$^{5)}$	3.26	F(20)	C(39)$^{1)}$	3.49(1)
F(20)	N(4)$^{1)}$	3.59(1)	F(20)	C(81)$^{6)}$	3.60(1)
F(20)	C(84)$^{6)}$	3.6215(8)	F(21)	O(16)$^{4)}$	3.61
F(21)	C(98)$^{4)}$	3.6333(1)	F(22)	H(53)$^{4)}$	2.77
F(22)	H(52)$^{4)}$	3.20	F(22)	C(70)$^{4)}$	3.33(1)
F(22)	C(69)$^{4)}$	3.57(1)	F(23)	H(53)$^{4)}$	2.34
F(23)	H(26)$^{5)}$	2.76	F(23)	C(70)$^{4)}$	3.16(1)
F(23)	C(46)$^{5)}$	3.20(1)	F(23)	N(7)$^{5)}$	3.43(1)
F(23)	H(52)$^{4)}$	3.66	F(24)	O(6)$^{5)}$	2.998(7)
F(24)	H(53)$^{4)}$	3.13	F(24)	H(26)$^{5)}$	3.16

Table 6. Non-bonded Contacts out to 3.80 $\AA$ (continued)

atom	atom	distance	atom	atom	distance
F(24)	C(46)$^{5)}$	3.35(2)	F(24)	H(12)$^{5)}$	3.53
F(24)	N(7)$^{5)}$	3.69(1)	F(25)	O(6)$^{5)}$	3.088(7)
F(25)	H(12)$^{5)}$	3.15	F(25)	C(99)$^{3)}$	3.3186(5)
F(25)	C(24)$^{5)}$	3.58(1)	F(27)	C(98)$^{4)}$	3.7444(2)
O(1)	C(102)$^{6)}$	3.394(7)	O(2)	C(102)$^{6)}$	3.551(7)
O(2)	H(61)$^{5)}$	3.67	O(3)	H(26)$^{5)}$	2.84
O(3)	C(46)$^{5)}$	3.37(1)	O(3)	N(7)$^{5)}$	3.40(1)
O(3)	H(53)$^{4)}$	3.44	O(3)	H(61)$^{5)}$	3.60
O(4)	H(45)$^{4)}$	3.21	O(4)	H(53)$^{4)}$	3.52
O(5)	H(35)$^{2)}$	2.66	O(5)	C(101)$^{1)}$	3.569(7)
O(5)	C(54)$^{2)}$	3.58(2)	O(5)	H(34)$^{2)}$	3.58
O(6)	H(54)$^{7)}$	3.65	O(6)	H(34)$^{2)}$	3.74
O(7)	H(22)$^{8)}$	2.55	O(7)	C(40)$^{8)}$	3.30(1)
O(7)	N(4)$^{8)}$	3.35(1)	O(8)	C(85)$^{9)}$	3.794(7)
O(9)	H(27)$^{3)}$	3.10	O(9)	H(21)$^{1)}$	3.48
O(9)	N(3)$^{1)}$	3.70(1)	O(10)	H(44)$^{4)}$	3.56
O(11)	H(21)$^{1)}$	2.41	O(11)	C(39)$^{1)}$	3.39(1)
O(13)	H(4)	2.40	O(13)	H(17)	2.61
O(13)	H(20)	2.71	O(13)	O(17)	3.19(1)
O(13)	C(8)	3.36(2)	O(13)	C(34)	3.51(2)
O(13)	H(3)	3.59	O(13)	C(38)	3.68(2)
O(14)	H(25)	2.49	O(14)	H(28)	2.76
O(14)	H(11)	2.78	O(14)	C(44)	3.41(2)
O(14)	C(48)	3.71(2)	O(14)	C(24)	3.72(2)

Table 6. Non-bonded Contacts out to 3.80 $\AA$ (continued)

atom	atom	distance	atom	atom	distance
O(15)	H(56)	2.66	O(15)	H(47)	2.81
O(15)	H(13)	2.86	O(15)	H(51)	3.27
O(15)	H(9)	3.31	O(15)	H(1)	3.34
O(15)	H(38)	3.35	O(15)	H(29)	3.60
O(15)	C(73)	3.60(1)	O(15)	H(5)	3.67
O(15)	C(68)	3.71(1)	O(15)	C(65)	3.74(1)
O(16)	H(33)$^{10)}$	3.04	O(16)	H(31)$^{10)}$	3.15
O(16)	C(52)$^{10)}$	3.44(1)	O(16)	C(50)$^{10)}$	3.69(1)
O(16)	H(32)$^{10)}$	3.72	O(16)	H(52)	3.73
O(16)	C(51)$^{10)}$	3.78(1)	O(17)	H(17)	3.06
O(17)	N(6)$^{6)}$	3.40(1)	O(17)	N(1)	3.59(1)
O(17)	H(20)	3.65	O(17)	C(93)	3.65(2)
O(17)	C(34)	3.67(1)	O(17)	C(94)$^{6)}$	3.67(3)
O(18)	N(6)$^{6)}$	3.15(1)	O(18)	C(43)$^{6)}$	3.24(1)
O(18)	H(24)$^{6)}$	3.38	O(18)	C(44)$^{6)}$	3.65(1)
O(18)	H(12)$^{6)}$	3.71	N(1)	C(94)$^{6)}$	3.47(3)
N(1)	N(8)$^{6)}$	3.72(1)	N(2)	C(88)$^{9)}$	3.39(2)
N(2)	C(86)$^{9)}$	3.50(2)	N(2)	C(87)$^{9)}$	3.66(2)
N(2)	C(83)$^{9)}$	3.77(2)	N(3)	H(24)$^{6)}$	2.50
N(3)	C(43)$^{6)}$	3.46(2)	N(3)	H(65)$^{11)}$	3.75
N(4)	H(15)$^{5)}$	2.72	N(4)	H(65)$^{11)}$	3.33
N(4)	C(32)$^{5)}$	3.44(2)	N(4)	C(47)$^{5)}$	3.47(2)
N(4)	N(8)$^{5)}$	3.55(2)	N(4)	N(7)$^{5)}$	3.64(2)
N(4)	C(48)$^{5)}$	3.65(2)	N(4)	C(46)$^{5)}$	3.74(2)

Table 6. Non-bonded Contacts out to 3.80 $\AA$ (continued)

atom	atom	distance	atom	atom	distance
N(4)	C(45)$^{5)}$	3.79(2)	N(6)	C(100)$^{1)}$	3.27(1)
N(6)	C(94)	3.57(3)	N(7)	H(8)$^{8)}$	2.55
N(7)	C(16)$^{8)}$	3.33(2)	N(7)	H(66)$^{8)}$	3.61
N(7)	C(40)$^{8)}$	3.68(2)	N(7)	C(87)$^{8)}$	3.73(2)
N(8)	H(18)$^{1)}$	2.39	N(8)	C(35)$^{1)}$	3.31(2)
N(8)	H(21)$^{8)}$	3.66	C(3)	C(98)$^{10)}$	3.79(1)
C(7)	H(62)$^{5)}$	3.37	C(8)	C(102)$^{6)}$	3.39(1)
C(9)	H(61)$^{5)}$	2.88	C(9)	H(62)$^{5)}$	3.61
C(9)	C(77)$^{5)}$	3.74(2)	C(10)	H(61)$^{5)}$	2.80
C(10)	C(77)$^{5)}$	3.77(2)	C(11)	H(61)$^{5)}$	2.84
C(11)	C(77)$^{5)}$	3.78(2)	C(12)	H(61)$^{5)}$	3.03
C(13)	H(61)$^{5)}$	3.11	C(13)	C(77)$^{5)}$	3.79(2)
C(14)	H(61)$^{5)}$	3.05	C(14)	H(62)$^{5)}$	3.34
C(14)	C(77)$^{5)}$	3.75(2)	C(15)	H(45)$^{4)}$	3.47
C(16)	H(26)$^{5)}$	3.35	C(16)	C(46)$^{5)}$	3.74(2)
C(17)	H(45)$^{4)}$	2.78	C(17)	C(63)$^{4)}$	3.77(2)
C(18)	H(45)$^{4)}$	3.28	C(19)	H(35)$^{2)}$	3.25
C(19)	H(45)$^{4)}$	3.67	C(19)	C(91)	3.78(2)
C(20)	H(45)$^{4)}$	3.66	C(20)	H(35)$^{2)}$	3.66
C(20)	C(91)	3.75(2)	C(21)	H(45)$^{4)}$	3.26
C(21)	C(91)	3.77(2)	C(22)	H(45)$^{4)}$	2.81
C(22)	C(63)$^{4)}$	3.77(2)	C(23)	H(35)$^{2)}$	3.69
C(24)	C(99)$^{1)}$	3.24(1)	C(24)	H(35)$^{2)}$	3.77
C(25)	H(54)$^{7)}$	2.94	C(25)	C(71)$^{7)}$	3.78(2)

Table 6. Non-bonded Contacts out to 3.80 $\AA$ (continued)

atom	atom	distance	atom	atom	distance
C(26)	H(54)$^{7)}$	3.10	C(27)	H(54)$^{7)}$	3.27
C(27)	H(22)$^{8)}$	3.61	C(28)	H(54)$^{7)}$	3.35
C(29)	H(54)$^{7)}$	3.17	C(29)	H(55)$^{7)}$	3.73
C(29)	C(91)	3.76(2)	C(30)	H(54)$^{7)}$	3.01
C(30)	C(91)	3.78(2)	C(30)	C(71)$^{7)}$	3.79(2)
C(32)	H(22)$^{8)}$	3.32	C(35)	H(27)$^{6)}$	3.41
C(35)	C(86)$^{9)}$	3.61(2)	C(35)	C(47)$^{6)}$	3.79(2)
C(36)	C(88)$^{9)}$	3.70(2)	C(36)	C(83)$^{9)}$	3.78(2)
C(37)	H(61)$^{5)}$	3.56	C(38)	H(24)$^{6)}$	3.70
C(39)	H(24)$^{6)}$	3.03	C(39)	H(65)$^{11)}$	3.41
C(39)	C(47)$^{5)}$	3.65(2)	C(39)	H(27)$^{5)}$	3.66
C(39)	H(15)$^{5)}$	3.77	C(40)	H(15)$^{5)}$	3.31
C(40)	H(61)$^{5)}$	3.48	C(40)	H(65)$^{11)}$	3.58
C(40)	C(46)$^{5)}$	3.63(2)	C(42)	H(44)$^{4)}$	3.66
C(43)	H(21)$^{1)}$	3.57	C(44)	C(94)	3.69(3)
C(44)	C(100)$^{1)}$	3.70(1)	C(45)	H(22)$^{8)}$	3.62
C(46)	H(8)$^{8)}$	3.21	C(46)	H(53)$^{7)}$	3.38
C(46)	H(22)$^{8)}$	3.40	C(47)	H(18)$^{1)}$	2.95
C(47)	H(8)$^{8)}$	3.59	C(47)	H(21)$^{8)}$	3.70
C(47)	H(66)$^{8)}$	3.75	C(48)	H(18)$^{1)}$	3.56
C(49)	H(62)$^{5)}$	3.20	C(49)	H(64)$^{10)}$	3.59
C(50)	H(59)$^{10)}$	3.32	C(50)	H(64)$^{10)}$	3.50
C(50)	H(57)$^{10)}$	3.78	C(51)	H(59)$^{10)}$	3.17
C(51)	H(62)$^{5)}$	3.58	C(51)	C(95)$^{10)}$	3.74(1)

Table 6. Non-bonded Contacts out to 3.80 $\AA$ (continued)

atom	atom	distance	atom	atom	distance
C(52)	C(95)$^{10)}$	3.60(1)	C(53)	C(102)$^{6)}$	3.69(2)
C(54)	H(50)$^{11)}$	3.25	C(54)	H(10)$^{11)}$	3.46
C(55)	H(50)$^{11)}$	3.32	C(55)	H(59)$^{10)}$	3.61
C(55)	H(62)$^{5)}$	3.63	C(55)	H(63)$^{5)}$	3.66
C(55)	C(61)$^{12)}$	3.70(2)	C(56)	H(59)$^{10)}$	2.81
C(56)	H(62)$^{5)}$	3.03	C(56)	H(64)$^{10)}$	3.35
C(56)	H(63)$^{5)}$	3.39	C(56)	C(74)$^{10)}$	3.67(2)
C(57)	H(46)$^{4)}$	3.41	C(59)	H(36)$^{12)}$	3.54
C(59)	H(49)$^{4)}$	3.72	C(60)	H(36)$^{12)}$	3.03
C(60)	H(63)$^{10)}$	3.05	C(61)	H(36)$^{12)}$	2.76
C(61)	H(63)$^{10)}$	3.00	C(61)	C(98)	3.56(2)
C(61)	C(79)$^{10)}$	3.59(2)	C(62)	H(36)$^{12)}$	3.05
C(62)	H(23)$^{4)}$	3.63	C(63)	H(49)$^{4)}$	3.24
C(63)	H(36)$^{12)}$	3.53	C(63)	H(39)$^{4)}$	3.64
C(64)	H(49)$^{4)}$	2.99	C(64)	H(39)$^{4)}$	3.27
C(64)	H(51)$^{4)}$	3.57	C(64)	C(66)$^{4)}$	3.75(2)
C(64)	C(68)$^{4)}$	3.77(2)	C(64)	H(36)$^{12)}$	3.79
C(65)	H(55)$^{7)}$	3.69	C(65)	C(95)	3.75(1)
C(66)	H(46)$^{4)}$	3.56	C(66)	H(35)$^{2)}$	3.80
C(67)	H(41)$^{4)}$	3.01	C(67)	H(46)$^{4)}$	3.43
C(68)	H(41)$^{4)}$	2.98	C(68)	H(46)$^{4)}$	3.05
C(68)	C(96)	3.60(1)	C(68)	C(95)	3.62(1)
C(68)	H(39)$^{4)}$	3.76	C(69)	H(41)$^{4)}$	3.04
C(69)	H(6)$^{4)}$	3.24	C(69)	H(39)$^{4)}$	3.62

Table 6. Non-bonded Contacts out to 3.80 $\AA$ (continued)

atom	atom	distance	atom	atom	distance
C(70)	H(41)$^{4)}$	3.09	C(70)	H(6)$^{4)}$	3.11
C(70)	H(26)$^{7)}$	3.26	C(71)	H(41)$^{4)}$	3.09
C(71)	H(60)$^{7)}$	3.22	C(71)	H(58)$^{7)}$	3.42
C(71)	H(26)$^{7)}$	3.52	C(71)	H(48)$^{7)}$	3.60
C(72)	H(41)$^{4)}$	3.08	C(72)	H(58)$^{7)}$	3.15
C(72)	H(48)$^{7)}$	3.21	C(72)	H(60)$^{7)}$	3.67
C(73)	H(32)$^{10)}$	3.32	C(74)	H(55)$^{7)}$	3.25
C(74)	H(37)$^{10)}$	3.26	C(74)	H(32)$^{10)}$	3.31
C(75)	H(37)$^{10)}$	3.26	C(76)	H(40)$^{8)}$	3.25
C(76)	H(54)$^{7)}$	3.69	C(76)	H(22)$^{8)}$	3.72
C(76)	H(41)$^{8)}$	3.74	C(77)	H(40)$^{8)}$	3.05
C(77)	H(22)$^{8)}$	3.41	C(77)	H(30)$^{8)}$	3.79
C(78)	H(30)$^{8)}$	3.11	C(78)	H(37)$^{8)}$	3.34
C(78)	H(43)$^{10)}$	3.60	C(78)	H(40)$^{8)}$	3.73
C(78)	H(42)$^{8)}$	3.78	C(79)	H(43)$^{10)}$	2.85
C(79)	H(63)$^{13)}$	3.28	C(79)	H(42)$^{10)}$	3.34
C(79)	H(37)$^{8)}$	3.34	C(79)	C(79)$^{13)}$	3.71(2)
C(79)	H(37)$^{10)}$	3.77	C(80)	H(37)$^{10)}$	2.87
C(80)	H(43)$^{10)}$	3.26	C(80)	H(63)$^{13)}$	3.43
C(80)	H(42)$^{10)}$	3.60	C(80)	H(32)$^{10)}$	3.71
C(81)	H(27)$^{3)}$	3.65	C(84)	H(27)$^{3)}$	3.53
C(85)	H(43)$^{4)}$	3.73	C(86)	H(21)$^{1)}$	3.27
C(89)	H(21)$^{1)}$	3.32	C(89)	H(27)$^{5)}$	3.72
C(90)	H(53)$^{4)}$	3.66	C(91)	H(11)	3.35

Table 6. Non-bonded Contacts out to 3.80 $\AA$ (continued)

atom	atom	distance	atom	atom	distance
C(91)	H(4)	3.47	C(91)	H(16)	3.63
C(91)	H(25)	3.71	C(91)	H(7)	3.76
C(92)	H(4)	3.26	C(92)	H(25)	3.34
C(92)	H(20)	3.49	C(92)	H(28)	3.50
C(92)	H(11)	3.53	C(92)	H(16)	3.57
C(92)	H(17)	3.59	C(93)	H(25)	3.09
C(93)	H(28)	3.30	C(94)	H(25)	3.07
C(94)	H(28)	3.32	C(95)	H(47)	3.19
C(95)	H(59)	3.33	C(95)	H(48)	3.38
C(95)	H(55)$^{7)}$	3.41	C(95)	H(50)$^{7)}$	3.63
C(95)	H(56)	3.63	C(95)	H(13)	3.69
C(95)	H(58)	3.69	C(96)	H(56)	3.13
C(96)	H(47)	3.23	C(96)	H(51)	3.45
C(96)	H(13)	3.53	C(96)	H(59)	3.69
C(97)	H(31)$^{10)}$	3.07	C(97)	H(33)$^{10)}$	3.43
C(98)	H(43)	3.19	C(98)	H(31)$^{10)}$	3.39
C(98)	H(57)$^{10)}$	3.42	C(98)	H(33)$^{10)}$	3.52
C(98)	H(19)$^{10)}$	3.67	C(99)	H(12)$^{6)}$	2.29
C(99)	H(66)$^{14)}$	2.80	C(99)	H(11)$^{6)}$	3.68
C(100)	H(12)$^{6)}$	3.10	C(100)	H(25)$^{6)}$	3.79
C(101)	H(12)$^{6)}$	3.49	C(101)	H(35)$^{1)}$	3.57
C(101)	H(34)$^{1)}$	3.59	C(102)	H(3)$^{1)}$	2.94
C(102)	H(34)$^{1)}$	3.47	C(102)	H(65)$^{6)}$	3.62
H(2)	H(62)$^{5)}$	3.06	H(5)	H(61)$^{5)}$	3.73

Table 6. Non-bonded Contacts out to 3.80 $\AA$ (continued)

atom	atom	distance	atom	atom	distance
H(6)	H(53)$^{4)}$	2.97	H(6)	H(52)$^{4)}$	3.17
H(6)	H(45)$^{4)}$	3.25	H(8)	H(26)$^{5)}$	3.03
H(8)	H(27)$^{5)}$	3.65	H(10)	H(35)$^{2)}$	2.94
H(10)	H(34)$^{2)}$	3.69	H(12)	H(34)$^{2)}$	3.72
H(12)	H(66)$^{8)}$	3.76	H(13)	H(55)$^{7)}$	3.58
H(13)	H(54)$^{7)}$	3.63	H(15)	H(22)$^{8)}$	3.06
H(18)	H(27)$^{6)}$	2.69	H(18)	H(28)$^{6)}$	3.77
H(21)	H(24)$^{6)}$	2.75	H(21)	H(27)$^{5)}$	3.62
H(21)	H(65)$^{11)}$	3.75	H(22)	H(61)$^{5)}$	2.81
H(22)	H(60)$^{5)}$	3.39	H(22)	H(26)$^{5)}$	3.42
H(23)	H(44)$^{4)}$	2.79	H(23)	H(45)$^{4)}$	3.42
H(26)	H(53)$^{7)}$	2.42	H(26)	H(54)$^{7)}$	3.05
H(29)	H(64)$^{10)}$	3.74	H(30)	H(62)$^{5)}$	2.46
H(30)	H(64)$^{10)}$	2.96	H(30)	H(61)$^{5)}$	3.76
H(32)	H(59)$^{10)}$	2.65	H(32)	H(57)$^{10)}$	2.81
H(32)	H(64)$^{10)}$	2.88	H(32)	H(56)$^{10)}$	3.32
H(35)	H(50)$^{11)}$	3.21	H(35)	H(49)$^{11)}$	3.55
H(36)	H(43)$^{12)}$	3.10	H(36)	H(63)$^{5)}$	3.24
H(36)	H(50)$^{11)}$	3.24	H(36)	H(42)$^{12)}$	3.39
H(36)	H(44)$^{12)}$	3.48	H(36)	H(49)$^{11)}$	3.59
H(36)	H(62)$^{5)}$	3.77	H(37)	H(64)$^{10)}$	2.41
H(37)	H(59)$^{10)}$	2.54	H(37)	H(63)$^{5)}$	2.70
H(37)	H(62)$^{5)}$	2.71	H(38)	H(46)$^{4)}$	3.75
H(39)	H(46)$^{4)}$	2.41	H(39)	H(45)$^{4)}$	3.14

Table 6. Non-bonded Contacts out to 3.80 $\AA$ (continued)

atom	atom	distance	atom	atom	distance
H(39)	H(52)$^{4)}$	3.50	H(39)	H(51)$^{4)}$	3.76
H(40)	H(61)$^{5)}$	3.00	H(40)	H(60)$^{5)}$	3.31
H(41)	H(60)$^{5)}$	3.44	H(41)	H(51)$^{4)}$	3.49
H(41)	H(52)$^{4)}$	3.57	H(41)	H(53)$^{4)}$	3.66
H(41)	H(55)$^{4)}$	3.67	H(41)	H(54)$^{4)}$	3.70
H(41)	H(49)$^{4)}$	3.80	H(42)	H(63)$^{10)}$	2.56
H(42)	H(64)$^{10)}$	3.13	H(43)	H(63)$^{10)}$	2.49
H(43)	H(64)$^{10)}$	3.25	H(45)	H(49)$^{4)}$	3.19
H(46)	H(51)$^{4)}$	2.71	H(46)	H(49)$^{4)}$	2.85
H(46)	H(46)$^{4)}$	2.90	H(48)	H(55)$^{7)}$	2.77
H(48)	H(54)$^{7)}$	3.46	H(48)	H(48)$^{7)}$	3.73
H(54)	H(60)$^{7)}$	2.78	H(54)	H(58)$^{7)}$	2.98
H(55)	H(58)$^{7)}$	2.45	H(55)	H(59)$^{7)}$	3.27
H(55)	H(60)$^{7)}$	3.61	H(63)	H(63)$^{13)}$	3.13
H(63)	H(64)$^{13)}$	3.41			

Symmetry operations

(1)	X,-Y+1/2,Z-1/2	(2)	X,Y,Z-1
(3)	X-1,-Y+1/2,Z-1/2	(4)	-X+2,-Y,-Z+2
(5)	X-1,Y,Z	(6)	X,-Y+1/2,Z+1/2
(7)	-X+3,-Y,-Z+2	(8)	X+1,Y,Z
(9)	X+1,Y,Z+1	(10)	-X+3,-Y,-Z+3
(11)	X,Y,Z+1	(12)	-X+2,-Y,-Z+3
(13)	-X+4,-Y,-Z+3	(14)	X+1,-Y+1/2,Z+1/2