checkCIF/PLATON report

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: 2

Bond precision: C-C = 0.0043 A Wavelength=0.71073

Cell: a=8.5296(14) b=8.8986(14) c=10.5757(15)
alpha=71.300(4) beta=78.698(4) gamma=74.264(5)
Temperature: 293 K

	Calculated	Reported
Volume	726.6(2)	726.59(19)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C30 H22 Mn N4 O6, 2(H2 O)	?
Sum formula	C30 H26 Mn N4 O8	C30 H26 Mn N4 O8
Mr	625.49	625.49
Dx,g cm-3	1.429	1.429
Z	1	1
Mu (mm-1)	0.512	0.512
F000	323.0	323.0
F000’	323.49	
h,k,lmax	10,10,12	10,10,12
Nref	2768	2748
Tmin,Tmax	0.912,0.950	0.878,0.951
Tmin’	0.875	

Correction method= # Reported T Limits: Tmin=0.878 Tmax=0.951
AbsCorr = MULTI-SCAN

Data completeness= 0.993 Theta(max)= 25.750

R(reflections)= 0.0591(2121) wR2(reflections)= 0.1541(2748)

S = 1.021 Npar= 196

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT245_ALERT_2_C	U(iso) H4A	Smaller than U(eq) O4	by ...	0.035	AngSq
PLAT245_ALERT_2_C	U(iso) H4B	Smaller than U(eq) O4	by ...	0.035	AngSq

Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF	Please	Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	4	Report
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	?	Check
PLAT093_ALERT_1_G	No s.u.'s on H-positions, Refinement Reported as	mixed	Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature ..... (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature ..... (K)	293	Check
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	1	Do !
	O1 -MN1 -O1 -C10 5.00 0.00 2.675 1.555 1.555 1.555		
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2014	Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
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9 **ALERT level G** = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

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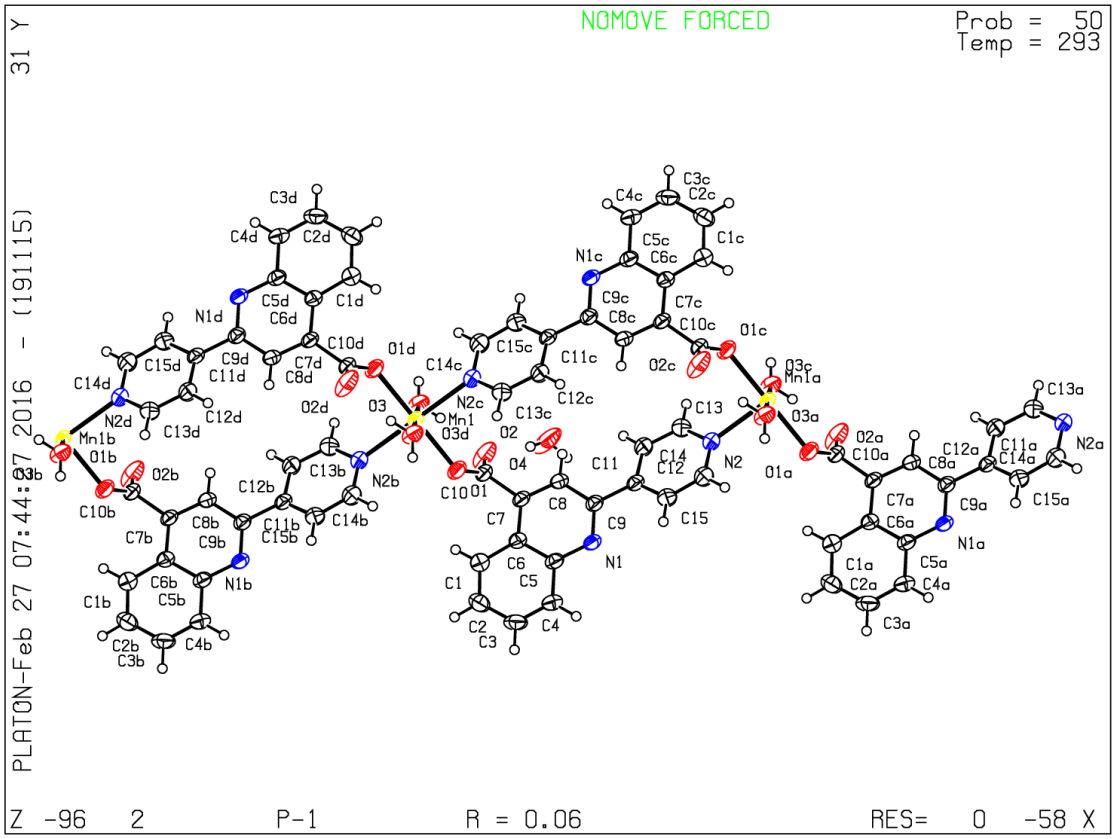
PLATON version of 19/11/2015; check.def file version of 17/11/2015

Datablock 2 - ellipsoid plot



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No syntax errors found. CIF dictionary Interpreting this report

Datablock: mo_qj_178_0m

```
Bond precision:  C-C = 0.0022 A          Wavelength=0.71073

Cell:          a=8.5511(4)       b=8.7942(5)      c=10.4459(5)
               alpha=70.748(2)   beta=78.982(1)   gamma=74.252(2)
Temperature:   293 K
```

	Calculated	Reported
Volume	709.29(6)	709.29(6)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C30 H22 Co N4 O6, 2(H2 O)	?
Sum formula	C30 H26 Co N4 O8	C30 H26 Co N4 O8
Mr	629.48	629.48
Dx,g cm-3	1.474	1.474
Z	1	1
Mu (mm-1)	0.664	0.664
F000	325.0	325.0
F000’	325.50	
h,k,lmax	10,10,12	10,10,12
Nref	2643	2607
Tmin,Tmax	0.819,0.905	0.826,0.907
Tmin’	0.819	

```
Correction method= # Reported T Limits: Tmin=0.826 Tmax=0.907
AbsCorr = MULTI-SCAN

Data completeness= 0.986          Theta(max)= 25.500

R(reflections)= 0.0279( 2468)     wR2(reflections)= 0.0733( 2607)

S = 1.108                 Npar= 196
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level G

```
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF      Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          4 Report
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as       mixed Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #          1 Do !
            O2  -CO1 -O2  -C10     7.00  0.00   2.557   1.555   1.555   1.555
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2014 Note
```

```
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```

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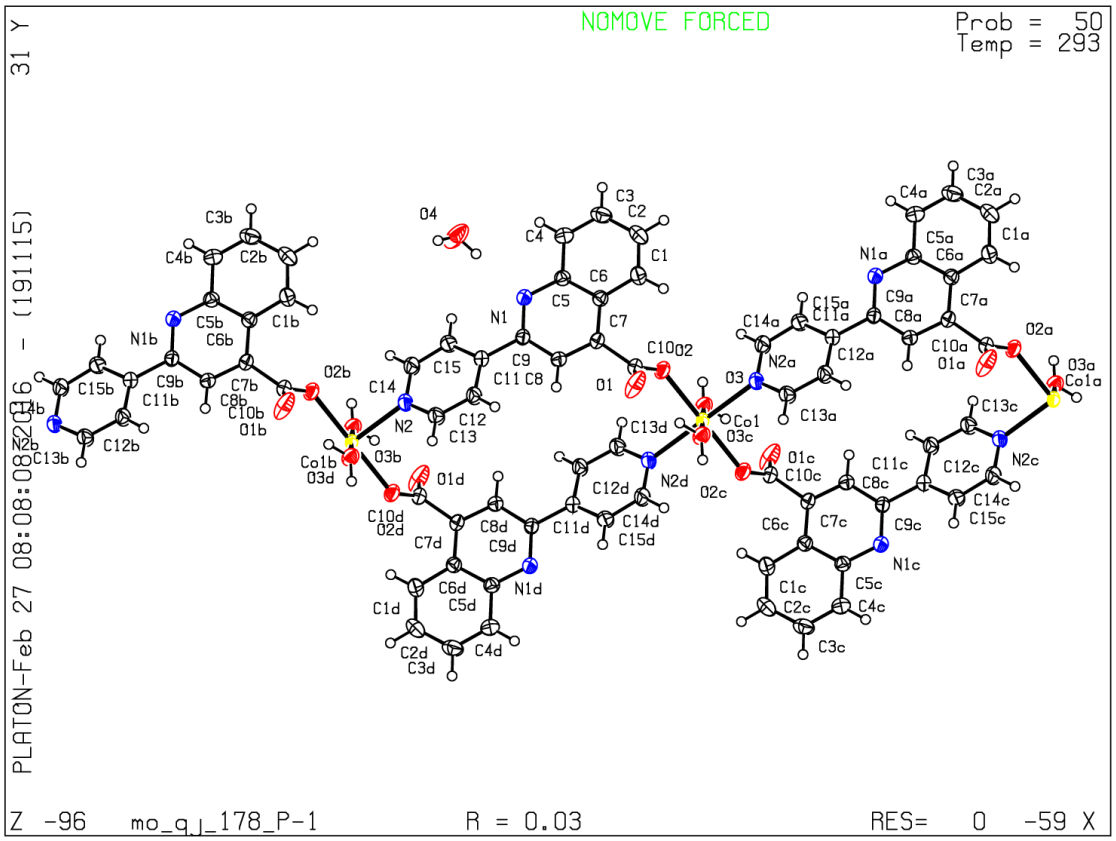
PLATON version of 19/11/2015; check.def file version of 17/11/2015

Datablock mo_qj_178_0m - ellipsoid plot



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No syntax errors found. CIF dictionary Interpreting this report

Datablock: 3

Bond precision: C-C = 0.0028 A Wavelength=0.71073

Cell: a=8.6281(5) b=8.9010(5) c=10.6287(7)
alpha=72.133(2) beta=78.500(2) gamma=74.632(1)
Temperature: 293 K

	Calculated	Reported
Volume	742.90(8)	742.90(8)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C30 H22 Cd N4 O6, 2(H2 O)	?
Sum formula	C30 H26 Cd N4 O8	C30 H26 Cd N4 O8
Mr	682.96	682.95
Dx,g cm-3	1.527	1.527
Z	1	1
Mu (mm-1)	0.791	0.791
F000	346.0	346.0
F000'	345.35	
h,k,lmax	10,10,13	10,10,13
Nref	2924	2877
Tmin,Tmax	0.827,0.924	0.821,0.925
Tmin'	0.814	

Correction method= # Reported T Limits: Tmin=0.821 Tmax=0.925
AbsCorr = MULTI-SCAN

Data completeness= 0.984 Theta(max)= 26.000

R(reflections)= 0.0218(2848) wR2(reflections)= 0.0569(2877)

S = 1.131 Npar= 196

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level G

```
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF      Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          4 Report
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as       mixed Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         44 Do !
            O1  -CD1 -O1  -C10     4.00  0.00   2.556   1.555   1.555   1.555
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2014 Note
```

```
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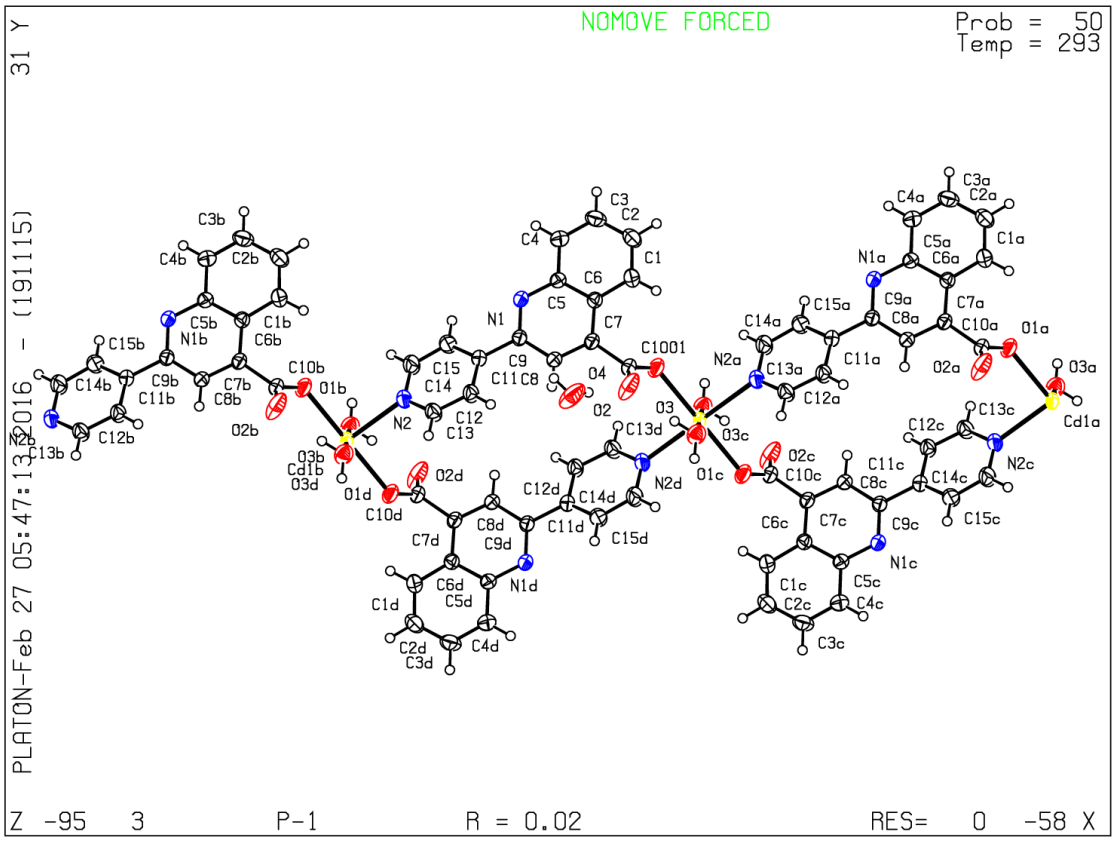
PLATON version of 19/11/2015; check.def file version of 17/11/2015

Datablock 3 - ellipsoid plot



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No syntax errors found. CIF dictionary Interpreting this report

Datablock: mm2

Bond precision: C-C = 0.0064 A Wavelength=0.71073

Cell: a=14.2981(7) b=17.5489(8) c=13.4398(7)
alpha=90 beta=114.657(1) gamma=90
Temperature: 298 K

	Calculated	Reported
Volume	3064.8(3)	3064.8(3)
Space group	C c	Cc
Hall group	C -2yc	?
Moiety formula	C30 H22 Ag2 N4 O6, 2(H O0.50), H O0.50, H2 O	?
Sum formula	C30 H28 Ag2 N4 O9	C30 H28 Ag2 N4 O9
Mr	804.30	804.30
Dx,g cm-3	1.743	1.743
Z	4	4
Mu (mm-1)	1.338	1.338
F000	1608.0	1608.0
F000’	1601.51	
h,k,lmax	18,22,17	18,22,17
Nref	7071[3541]	6509
Tmin,Tmax	0.733,0.875	0.732,0.874
Tmin’	0.709	

Correction method= # Reported T Limits: Tmin=0.732 Tmax=0.874
AbsCorr = MULTI-SCAN

Data completeness= 1.84/0.92 Theta(max)= 27.540

R(reflections)= 0.0362(6051) wR2(reflections)= 0.0949(6509)

S = 1.054 Npar= 413

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT420_ALERT_2_B	D-H Without Acceptor	*O8	--	*H8A	...	Please Check

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Alert level C

PLAT090_ALERT_3_C	Poor Data / Parameter Ratio (Zmax > 18)					8.57 Note
PLAT165_ALERT_3_C	Nr. of Status R Flagged Non-Hydrogen Atoms					1 Note
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of					C10 Check
PLAT245_ALERT_2_C	U(iso) H6A	Smaller than U(eq) O6			by ...	0.021 AngSq
PLAT245_ALERT_2_C	U(iso) H6B	Smaller than U(eq) O6			by ...	0.021 AngSq
PLAT314_ALERT_2_C	Check Small Angle for H2O: Metal-O6			-H6B		83.20 Degree
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond	C7	-	C10	..	1.53 Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported	H8A	..	O1	..	2.65 Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported	H6B	..	O5	..	2.64 Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported	H5B	..	O6	..	2.61 Ang.

Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension					3 Info
PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF					Please Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms					12 Report
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical					? Check
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Ag1	--	O5	..	12.5 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Ag1	--	O6	..	7.0 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Ag1	--	N1	..	16.1 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Ag1	--	N3	..	8.3 s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of *O8			is Constrained at		0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *H8A			is Constrained at		0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *H8B			is Constrained at		0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *O9			is Constrained at		0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *H9A			is Constrained at		0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *H9B			is Constrained at		0.5 Check
PLAT302_ALERT_4_G	Anion/Solvent Disorder ..... Percentage =					33 Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL					2014 Note

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PLATON version of 08/07/2016; check.def file version of 05/07/2016

Datablock mm2 - ellipsoid plot