checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 1

```
Bond precision:  C-C = 0.0060 A          Wavelength=0.71073

Cell:          a=8.6450(17)      b=9.5075(17)     c=10.8250(18)
               alpha=82.180(5)   beta=88.184(6)   gamma=89.803(6)
Temperature:   293 K
```

	Calculated	Reported
Volume	881.0(3)	881.0(3)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C12 H14 Mn N5 O6, N O3	?
Sum formula	C12 H14 Mn N6 O9	C12 H14 Mn N6 O9
Mr	441.23	441.23
Dx,g cm-3	1.663	1.663
Z	2	2
Mu (mm-1)	0.812	0.812
F000	450.0	450.0
F000’	450.91	
h,k,lmax	10,11,12	10,11,12
Nref	3129	3125
Tmin,Tmax	0.850,0.885	0.854,0.888
Tmin’	0.850	

```
Correction method= ?

Data completeness= 0.999          Theta(max)= 25.040

R(reflections)= 0.0529( 2293)     wR2(reflections)= 0.1667( 3125)

S = 1.052                 Npar= 269
```

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

PLAT052_ALERT_1_C	Info on Absorption Correction Method Not Given .	Please Do !
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.01 Report
PLAT230_ALERT_2_C	Hirshfeld Test Diff for O2 -- N5 ..	5.7 su
PLAT230_ALERT_2_C	Hirshfeld Test Diff for O3 -- N5 ..	6.0 su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X) Mn1 -- O2 ..	7.2 su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X) Mn1 -- O3 ..	9.0 su
PLAT241_ALERT_2_C	High Ueq as Compared to Neighbors for	O3 Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	N6 Check

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	6 Note
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF	Please Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1 Report
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	? Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large.	0.11 Report
PLAT180_ALERT_4_G	Check Cell Rounding: # of Values Ending with 0 =	3
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature ..... (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature ..... (K)	293 Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	6 Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2014 Note

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
10 **ALERT level G** = General information/check it is not something unexpected

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

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

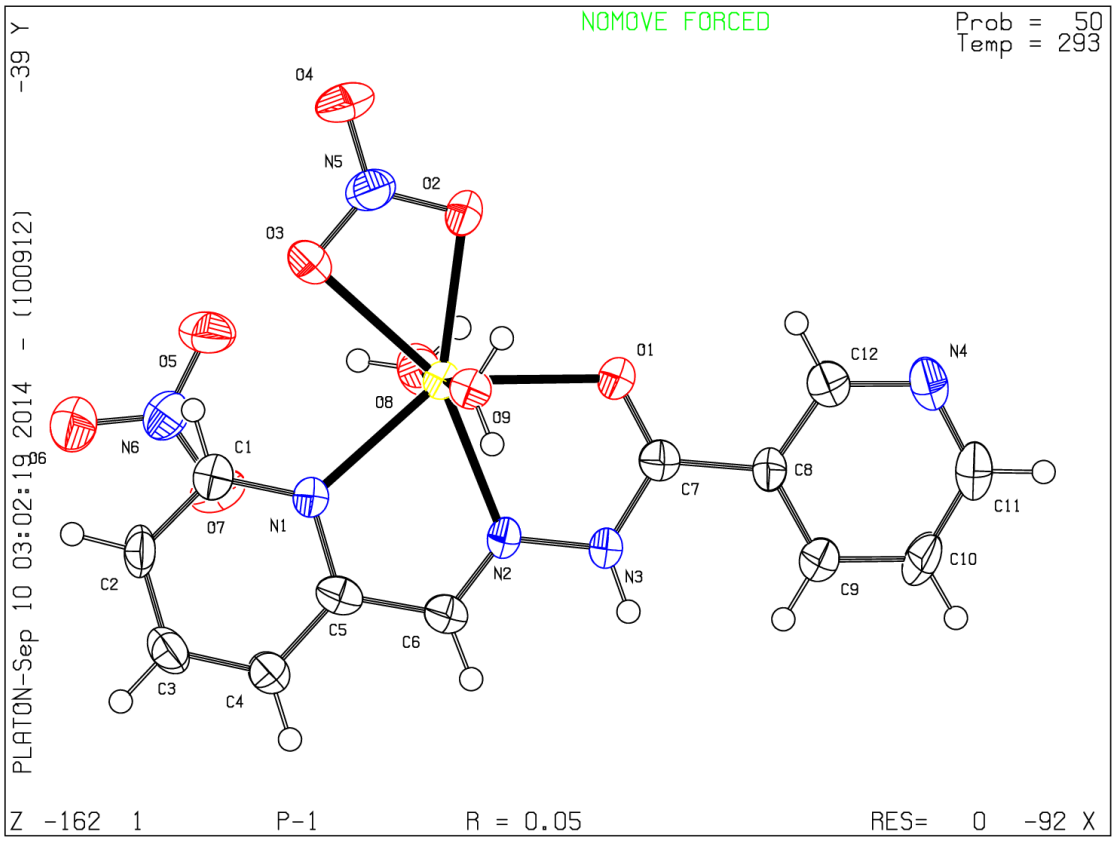
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 20/08/2014; check.def file version of 18/08/2014

Datablock 1 - ellipsoid plot



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Datablock: 2

Bond precision: C-C = 0.0033 A Wavelength=0.71073

Cell: a=9.1500(4) b=10.4018(5) c=14.4785(6)
alpha=83.173(1) beta=86.514(1) gamma=89.360(2)
Temperature: 293 K

	Calculated	Reported
Volume	1365.70(11)	1365.70(11)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C24 H22 Mn N9 O6, N O3	?
Sum formula	C24 H22 Mn N10 O9	C24 H22 Mn N10 O9
Mr	649.46	649.46
Dx,g cm-3	1.579	1.579
Z	2	2
Mu (mm-1)	0.556	0.556
F000	666.0	666.0
F000’	666.97	
h,k,lmax	11,13,18	11,13,18
Nref	6318	6161
Tmin,Tmax	0.885,0.905	0.887,0.906
Tmin’	0.885	

Correction method= ?

Data completeness= 0.975 Theta(max)= 27.570

R(reflections)= 0.0448(4737) wR2(reflections)= 0.1217(6161)

S = 1.027 Npar= 414

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test-name_ALERT_alert-type_alert-level.
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Alert level C

PLAT029_ALERT_3_C	_diffrn_measured_fraction_theta_full Low	0.974 Note
PLAT052_ALERT_1_C	Info on Absorption Correction Method Not Given .	Please Do !
PLAT241_ALERT_2_C	High Ueq as Compared to Neighbors for	O3 Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for	Mn1 Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for	N8 Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	N9 Check

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Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	4 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	5 Report
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF	Please Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	2 Report
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	? Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature ..... (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature ..... (K)	293 Check
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Mn1 -- O1 ..	7.2 su
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Mn1 -- O3 ..	18.9 su
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Mn1 -- N6 ..	5.8 su
PLAT301_ALERT_3_G	Main Residue Disorder ..... Percentage =	3 Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	63 Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2014 Note

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Datablock 2 - ellipsoid plot