checkCIF/PLATON report

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

No syntax errors found. CIF dictionary Interpreting this report

Datablock: I

Bond precision: C-C = 0.0156 A Wavelength=0.71069

Cell: a=12.6053(9) b=20.6331(16) c=15.5228(12)
alpha=90 beta=96.134(7) gamma=90
Temperature: 110 K

	Calculated	Reported
Volume	4014.2(5)	4014.1(5)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	C76 H92 Mn6 N6 O26	C76 H92 Mn6 N6 O26
Sum formula	C76 H92 Mn6 N6 O26	C76 H92 Mn6 N6 O26
Mr	1835.20	1835.16
Dx,g cm-3	1.518	1.518
Z	2	2
Mu (mm-1)	0.997	0.997
F000	1896.0	1896.0
F000’	1900.87	
h,k,lmax	17,28,21	17,28,21
Nref	11667[22739]	19000
Tmin,Tmax	0.898,0.932	0.820,0.930
Tmin’	0.776	

Correction method= ANALYTICAL

Data completeness= 1.63/0.84 Theta(max)= 29.684

R(reflections)= 0.0727(11223) wR2(reflections)= wR= 0.0846(11223)

S = 1.095 Npar= 1028

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.

[IMAGE] **Alert level B**

PLAT220_ALERT_2_B Large Non-Solvent C Ueq(max)/Ueq(min) ... 5.5 Ratio
PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.0156 Ang
PLAT413_ALERT_2_B Short Inter XH3 .. XHn H1501 .. H261 .. 2.02 Ang.

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PLAT413_ALERT_2_B Short Inter XH3 .. XHn     H2032  ..  H841    ..       2.00 Ang.
PLAT420_ALERT_2_B D-H Without Acceptor       O125   -   H1252  ...         ?
PLAT420_ALERT_2_B D-H Without Acceptor       O145   -   H1452  ...         ?
PLAT420_ALERT_2_B D-H Without Acceptor       O201   -   H102   ...         ?
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[IMAGE] **Alert level C**

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PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low .......      0.973
PLAT213_ALERT_2_C Atom C6              has ADP max/min Ratio .....        3.4 prola
PLAT222_ALERT_3_C Large Non-Solvent    H    Uiso(max)/Uiso(min) ..        5.3 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference O211   --  C212    ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C212   --  C213    ..       0.18 Ang.
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for         O1
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for       C128
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for       C148
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        Mn5
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C172   -   C173   ...       1.42 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C212   -   C213   ...       1.41 Ang.
PLAT415_ALERT_2_C Short Inter D-H..H-X       H1252  ..  H891    ..       2.13 Ang.
PLAT416_ALERT_2_C Short Intra D-H..H-D       H104   ..  H105    ..       1.97 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          1
             C76 H92 Mn6 N6 O26
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[IMAGE] **Alert level G**

```
REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is
           correct. If it is not, please give the correct count in the
           _publ_section_exptl_refinement section of the submitted CIF.
          From the CIF: _diffrn_reflns_theta_max          29.68
          From the CIF: _reflns_number_total             19000
          Count of symmetry unique reflns        11667
          Completeness (_total/calc)            162.85%
          TEST3: Check Friedels for noncentro structure
          Estimate of Friedel pairs measured      7333
          Fraction of Friedel pairs measured     0.629
          Are heavy atom types Z>Si present         yes
PLAT007_ALERT_5_G Note: Number of Unrefined D-H Atoms .....          8
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Mn4    --  O121    ..       5.7 su
PLAT432_ALERT_2_G Short Inter X...Y Contact  C7     ..  C63     ..      3.18 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C23    ..  C107    ..      3.17 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....         51
PLAT791_ALERT_4_G Note: The Model has Chirality at C124   (Verify)         S
PLAT791_ALERT_4_G Note: The Model has Chirality at C144   (Verify)         S
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found         !
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......        97
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   7 ALERT level B = A potentially serious problem, consider carefully
  14 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

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

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 21/12/2011; check.def file version of 16/12/2011

Datablock I - ellipsoid plot

[IMAGE]