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: MnGd

```
Bond precision:  C-C = 0.0192 A          Wavelength=0.71073

Cell:          a=12.9744(11)     b=13.1470(9)     c=13.1693(11)
               alpha=86.455(6)   beta=77.910(7)   gamma=66.666(7)
Temperature:   150 K
```

	Calculated	Reported
Volume	2016.3(3)	2016.3(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C50 H90 Gd2 Mn2 O22, 2(C6 H16 N), 0.666(H2 O)	C50 H90 Gd2 Mn2 O22, 2(C6 H16 N), 0.67(H2 O)
Sum formula	C62 H123.33 Gd2 Mn2 N2 O22.67	C62 H123.33 Gd2 Mn2 N2 O22.67
Mr	1683.99	1684.05
Dx,g cm-3	1.387	1.387
Z	1	1
Mu (mm-1)	1.994	1.994
F000	868.7	869.0
F000’	869.35	
h,k,lmax	15,15,15	15,15,15
Nref	6882	6812
Tmin,Tmax	0.953,0.980	0.801,1.000
Tmin’	0.942	

```
Correction method= # Reported T Limits: Tmin=0.801 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.990          Theta(max)= 24.712

R(reflections)= 0.0813( 3900)     wR2(reflections)= 0.1423( 6812)

S = 1.024                 Npar= 436
```

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

```
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
          Calculated sin(theta_max)/wavelength =    0.5882
PLAT077_ALERT_4_C Unitcell contains non-integer number of atoms ..     Please Check
PLAT213_ALERT_2_C Atom C3             has ADP max/min Ratio .....        3.1 prolat
PLAT213_ALERT_2_C Atom C23            has ADP max/min Ratio .....        3.7 prolat
PLAT220_ALERT_2_C Large Non-Solvent  C     Ueq(max)/Ueq(min) Range       3.6 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference Gd1    --  C21     ..       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C17    --  C19     ..       0.18 Ang.
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....         O9 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        Gd1 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....         C2 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....         C7 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        C12 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        C17 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.5 Note
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.0192 Ang.
```

Alert level G

```
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          4 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          3 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT300_ALERT_4_G Atom Site Occupancy of <O12    is Constrained at      0.333 Check
PLAT302_ALERT_4_G Anion/Solvent Disorder ..... Percentage =             5 Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.24 Ratio
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #          3 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2 Note
            C6 H16 N
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         24 Note
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  15 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

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  11 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
   8 ALERT type 4 Improvement, methodology, query or suggestion
   1 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 29/01/2015; check.def file version of 29/01/2015

Datablock MnGd - ellipsoid plot