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: MgGd

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Bond precision:  C-C = 0.0101 A          Wavelength=0.71073

Cell:           a=15.7351(8)    b=13.1771(6)        c=21.9189(11)
                alpha=90        beta=109.951(6)     gamma=90
Temperature:    150 K
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	Calculated	Reported
Volume	4272.0(4)	4272.0(4)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C50 H90 Gd2 Mg2 O22, 2(C6 H16 N), C2 H3 N	C50 H90 Gd2 Mg2 O22, 2(C6 H16 N), C2 H3 N
Sum formula	C64 H125 Gd2 Mg2 N3 O22	C64 H125 Gd2 Mg2 N3 O22
Mr	1651.79	1651.78
Dx,g cm-3	1.284	1.284
Z	2	2
Mu (mm-1)	1.616	1.616
F000	1716.0	1716.0
F000’	1716.18	
h,k,lmax	19,16,27	19,16,27
Nref	8746	8731
Tmin,Tmax	0.731,0.785	0.655,1.000
Tmin’	0.717	

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Correction method= # Reported T Limits: Tmin=0.655 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 26.372

R(reflections)= 0.0502( 6964)     wR2(reflections)= 0.1326( 8731)

S = 1.053                 Npar= 492
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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

PLAT213_ALERT_2_C Atom C18 has ADP max/min Ratio ..... 3.1 prolat
PLAT213_ALERT_2_C Atom C20 has ADP max/min Ratio ..... 3.8 prolat
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) Range 5.5 Ratio
PLAT223_ALERT_4_C Large Solvent/Anion H Ueq(max)/Ueq(min) ..... 3.3 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C29 -- C31 .. 0.21 Ang.
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C2 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
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of N1 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C29 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0101 Ang.

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 12 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 3 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 2 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 3 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 10 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 1 Report
PLAT231_ALERT_4_G Hirshfeld Test (Solvent) C29 -- C30B .. 5.1 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Gd1 -- O1 .. 9.0 su
PLAT300_ALERT_4_G Atom Site Occupancy of >O11 is Constrained at 0.661 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <O11B is Constrained at 0.339 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C1 is Constrained at 0.661 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C3 is Constrained at 0.661 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C4 is Constrained at 0.661 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C1B is Constrained at 0.339 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C3B is Constrained at 0.339 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C4B is Constrained at 0.339 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >O11_a is Constrained at 0.661 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <O11B_a is Constrained at 0.339 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C1_a is Constrained at 0.661 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C3_a is Constrained at 0.661 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C4_a is Constrained at 0.661 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C1B_a is Constrained at 0.339 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C3B_a is Constrained at 0.339 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C4B_a is Constrained at 0.339 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C28 is Constrained at 0.661 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C30 is Constrained at 0.661 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C31 is Constrained at 0.661 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C1L is Constrained at 0.339 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C30B is Constrained at 0.339 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C31B is Constrained at 0.339 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *N2 is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C32 is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C33 is Constrained at 0.500 Check
PLAT301_ALERT_3_G Main Residue Disorder ..... Percentage = 11 Note
PLAT302_ALERT_4_G Anion/Solvent Disorder ..... Percentage = 53 Note
PLAT432_ALERT_2_G Short Inter X...Y Contact O9 .. C30B .. 2.99 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact C28 .. C33 .. 3.09 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 10 Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.15 Ratio
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 29 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
 11 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 40 ALERT level G = General information/check it is not something unexpected

  0 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
 36 ALERT type 4 Improvement, methodology, query or suggestion
  1 ALERT type 5 Informative message, check
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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 MgGd - ellipsoid plot