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: CoGd

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Bond precision:  C-C = 0.0068 A          Wavelength=0.71073

Cell:           a=15.7469(4)    b=13.0245(2)        c=21.9609(5)
                alpha=90        beta=110.893(3)     gamma=90
Temperature:    101 K
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	Calculated	Reported
Volume	4207.93(18)	4207.91(18)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C50 H90 Co2 Gd2 O22, 2(C6 H16 N), C2 N	C50 H90 Co2 Gd2 O22, 2(C6 H16 N), C2 N
Sum formula	C64 H122 Co2 Gd2 N3 O22	C64 H122 Co2 Gd2 N3 O22
Mr	1718.01	1718.00
Dx,g cm-3	1.356	1.356
Z	2	2
Mu (mm-1)	2.006	2.006
F000	1770.0	1770.0
F000’	1771.43	
h,k,lmax	19,16,27	19,16,27
Nref	8615	8600
Tmin,Tmax	0.786,0.852	0.652,1.000
Tmin’	0.770	

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Correction method= # Reported T Limits: Tmin=0.652 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 26.372

R(reflections)= 0.0345( 7604)     wR2(reflections)= 0.0947( 8600)

S = 1.060                 Npar= 519
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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 B

PLAT223_ALERT_4_B Large Solvent/Anion H Ueq(max)/Ueq(min) ..... 4.4 Ratio
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Gd1 -- O1 .. 15.2 su

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Alert level C

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.31 Report
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) Range 3.7 Ratio
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... O1 Check
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... O2 Check
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... O9 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 ..... C17 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of N11 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C29 Check
PLAT413_ALERT_2_C Short Inter XH3 .. XHn H5A .. H5AB .. 2.05 Ang.

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 5 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 10 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 2 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large. 8.90 Why ?
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 1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 1 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for C7 -- C8 .. 9.3 su
PLAT230_ALERT_2_G Hirshfeld Test Diff for C7 -- C9 .. 6.0 su
PLAT231_ALERT_4_G Hirshfeld Test (Solvent) C29 -- C30 .. 8.9 su
PLAT231_ALERT_4_G Hirshfeld Test (Solvent) C29 -- C30A .. 8.1 su
PLAT300_ALERT_4_G Atom Site Occupancy of >O11 is Constrained at 0.696 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <O13 is Constrained at 0.304 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C1 is Constrained at 0.696 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C3 is Constrained at 0.728 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C4 is Constrained at 0.728 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C8 is Constrained at 0.758 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C9 is Constrained at 0.758 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C10 is Constrained at 0.758 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C0AA is Constrained at 0.304 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C1AA is Constrained at 0.272 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C2AA is Constrained at 0.272 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C3AA is Constrained at 0.242 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C4AA is Constrained at 0.242 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C5AA is Constrained at 0.242 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >O11_a is Constrained at 0.696 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <O13_a is Constrained at 0.304 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C1_a is Constrained at 0.696 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C3_a is Constrained at 0.728 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C4_a is Constrained at 0.728 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C8_a is Constrained at 0.758 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C9_a is Constrained at 0.758 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C10_a is Constrained at 0.758 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C0AA_a is Constrained at 0.304 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C1AA_a is Constrained at 0.272 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C2AA_a is Constrained at 0.272 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C3AA_a is Constrained at 0.242 Check

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PLAT300_ALERT_4_G Atom Site Occupancy of <C4AA_a is Constrained at      0.242 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C5AA_a is Constrained at      0.242 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C26A   is Constrained at      0.532 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C30    is Constrained at      0.626 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C31    is Constrained at      0.626 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C27    is Constrained at      0.468 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C30A   is Constrained at      0.374 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C31A   is Constrained at      0.374 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *N1     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 =         18 Note
PLAT302_ALERT_4_G Anion/Solvent Disorder ..... Percentage =         53 Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   1.50) in Resd. #          3 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....         21 Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.14 Ratio
PLAT793_ALERT_4_G The Model has Chirality at C11     (Centro SPGR)          R Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....         62 Note
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   2 ALERT level B = A potentially serious problem, consider carefully
  10 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  55 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  14 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 ALERT type 3 Indicator that the structure quality may be low
  50 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 CoGd - ellipsoid plot