

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ata520c\_0m

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: ata520c\_0m

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Bond precision:	C-C = 0.0130 A	Wavelength=0.71073
Cell:	a=18.9025(5)	b=18.9025(5)      c=12.2959(6)
	alpha=90	beta=90      gamma=90
Temperature:	173 K	
	Calculated	Reported
Volume	4393.4(3)	4393.4(5)
Space group	P 4/n	P 4/n
Hall group	-P 4a	-P 4a
Moiety formula	C <sub>48</sub> H <sub>52</sub> Gd Mn <sub>4</sub> N <sub>4</sub> O <sub>20</sub> , C <sub>16</sub> H <sub>36</sub> N, 4(C H <sub>2</sub> Cl <sub>2</sub> ), C H <sub>2</sub> Cl, Cl	C <sub>48</sub> H <sub>52</sub> Gd Mn <sub>4</sub> N <sub>4</sub> O <sub>20</sub> , 5(C H <sub>2</sub> Cl <sub>2</sub> ), C <sub>16</sub> H <sub>36</sub> N
Sum formula	C <sub>69</sub> H <sub>98</sub> Cl <sub>10</sub> Gd Mn <sub>4</sub> N <sub>5</sub> O <sub>20</sub>	C <sub>69</sub> H <sub>98</sub> Cl <sub>10</sub> Gd Mn <sub>4</sub> N <sub>5</sub> O <sub>20</sub>
Mr	2049.03	2049.03
Dx, g cm <sup>-3</sup>	1.549	1.549
Z	2	2
Mu (mm <sup>-1</sup> )	1.674	1.674
F000	2082.0	2082.0
F000'	2088.03	
h,k,lmax	22,22,14	22,22,14
Nref	3881	3880
Tmin,Tmax	0.452,0.920	0.601,0.746
Tmin'	0.429	

Correction method= # Reported T Limits: Tmin=0.601 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 1.000      Theta(max)= 25.000

R(reflections)= 0.0431( 3426)      wR2(reflections)= 0.1077( 3880)

S = 1.240      Npar= 447

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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

PLAT220\_ALERT\_2\_B Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 7.5 Ratio

**Author Response: The metallocrowns can be arranged clockwise [M-NO-M] or anticlockwise [M-ON-M], with slightly different position for the transition metal ions, while the central lanthanide ions remains on its position in both isomers. The site occupation factor of the isomers were refined free to 0.82/0.18. Due to the large difference in site occupation factor a large Ueq(max)/Ueq(min) range can be observed.**



#### Alert level C

PLAT088\_ALERT\_3\_C Poor Data / Parameter Ratio ..... 8.68 Note  
PLAT222\_ALERT\_3\_C Non-Solv. Resd 1 H Uiso(max)/Uiso(min) Range 9.0 Ratio  
PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of C14 Check  
PLAT244\_ALERT\_4\_C Low 'Solvent' Ueq as Compared to Neighbors of C17 Check  
PLAT342\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.013 Ang.  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 2.535 Check  
PLAT934\_ALERT\_3\_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers .... 1 Check



#### Alert level G

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 17 Note  
PLAT003\_ALERT\_2\_G Number of Uiso or Uij Restrained non-H Atoms ... 22 Report  
PLAT042\_ALERT\_1\_G Calc. and Reported MoietyFormula Strings Differ Please Check  
PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large 17.77 Why ?  
PLAT152\_ALERT\_1\_G The Supplied and Calc. Volume s.u. Differ by ... -2 Units  
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 2 Report  
PLAT176\_ALERT\_4\_G The CIF-Embedded .res File Contains SADI Records 3 Report  
PLAT186\_ALERT\_4\_G The CIF-Embedded .res File Contains ISOR Records 6 Report  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of C15 Constrained at 0.6 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of C16 Constrained at 0.6 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of C15A Constrained at 0.4 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of C16A Constrained at 0.4 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H14A Constrained at 0.6 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H14B Constrained at 0.6 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H15A Constrained at 0.6 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H15B Constrained at 0.6 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H16A Constrained at 0.6 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H16B Constrained at 0.6 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H16C Constrained at 0.6 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H14C Constrained at 0.4 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H14D Constrained at 0.4 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H15C Constrained at 0.4 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H15D Constrained at 0.4 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H16D Constrained at 0.4 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H16E Constrained at 0.4 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H16F Constrained at 0.4 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of C13 Constrained at 0.25 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of C18 Constrained at 0.25 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H18A Constrained at 0.25 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H18B Constrained at 0.25 Check



PLAT300_ALERT_4_G	Atom Site Occupancy of Cl4	Constrained at	0.25	Check
PLAT301_ALERT_3_G	Main Residue Disorder .....	(Resd 1 )	99%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 2 )	47%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 4 )	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 5 )	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in .....	Resd 5	0.25	Check
PLAT780_ALERT_1_G	Coordinates do not Form a Properly Connected Set			Please Do !
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #		5	Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms ....			! Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....		175	Note
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still		76%	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF ....		1	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		1	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		1	Info

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 7 ALERT type 2 Indicator that the structure model may be wrong or deficient  
 9 ALERT type 3 Indicator that the structure quality may be low  
 33 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* or *IUCrData*, 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 23/04/2018; check.def file version of 23/04/2018

Datablock ata520c\_0m - ellipsoid plot

