

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) gvs1014c\_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: gvs1014c\_0m

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Bond precision:	C-C = 0.0192 Å	Wavelength=1.54178
Cell:	a=10.5235(15)	b=18.133(3)      c=19.488(3)
	alpha=90	beta=96.944(12)      gamma=90
Temperature:	173 K	
	Calculated	Reported
Volume	3691.5(10)	3691.6(9)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C60 H60 N10 O26 P4 Sm2, 2(H2 O)	C60 H60 N10 O26 P4 Sm2, 2(H2 O)
Sum formula	C60 H64 N10 O28 P4 Sm2	C60 H64 N10 O28 P4 Sm2
Mr	1797.81	1797.79
Dx,g cm-3	1.617	1.617
Z	2	2
Mu (mm-1)	13.393	13.393
F000	1804.0	1804.0
F000'	1791.13	
h,k,lmax	12,22,23	12,22,23
Nref	7211	6996
Tmin,Tmax	0.165,0.430	0.486,0.753
Tmin'	0.024	

Correction method= # Reported T Limits: Tmin=0.486 Tmax=0.753  
AbsCorr = MULTI-SCAN

Data completeness= 0.970      Theta(max)= 71.720

R(reflections)= 0.0722( 3911)      wR2(reflections)= 0.1815( 6996)

S = 1.020      Npar= 472

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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

PLAT241\_ALERT\_2\_B High 'MainMol' Ueq as Compared to Neighbors of 09 Check

**Author Response:** This atom assignment was confirmed as an oxygen (of a nitrate group). O9 is bonded directly to the Sm metal center (which has a relatively small U(eq) value). This difference is likely what triggered this alert.



#### Alert level C

RINTA01\_ALERT\_3\_C The value of Rint is greater than 0.12  
Rint given 0.146  
PLAT020\_ALERT\_3\_C The Value of Rint is Greater Than 0.12 ..... 0.146 Report  
PLAT220\_ALERT\_2\_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.6 Ratio  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference Sm1 --O12 . 0.16 Ang.  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference P1 --C11 . 0.16 Ang.  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C11 --C12 . 0.16 Ang.  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C11 --C16 . 0.16 Ang.  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C14 --C15 . 0.21 Ang.  
PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of 05 Check

**Author Response:** This atom assignment was confirmed as an oxygen (of a nitrate group). O9 is bonded directly to the Sm metal center (which has a relatively small U(eq) value). This difference is likely what triggered this alert.

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of 06 Check

**Author Response:** This atom assignment was confirmed as an oxygen (of a nitrate group). O9 is bonded directly to the Sm metal center (which has a relatively small U(eq) value). This difference is likely what triggered this alert.

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of 012 Check

**Author Response:** This atom assignment was confirmed as an oxygen (of a nitrate group). O9 is bonded directly to the Sm metal center (which has a relatively small U(eq) value). This difference is likely what triggered this alert.

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of C9 Check

**Author Response:** This atom assignment was confirmed as an oxygen (of a nitrate group). O9 is bonded directly to the Sm metal center (which has a relatively small U(eq) value). This difference is likely what triggered this alert.

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of C18 Check

**Author Response:** This atom assignment was confirmed as an oxygen (of a nitrate group). O9 is bonded directly to the Sm metal center (which has a relatively small U(eq) value). This difference is likely what triggered this alert.

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of C28 Check

**Author Response:** This atom assignment was confirmed as an oxygen (of a nitrate group). O9 is bonded directly to the Sm metal center (which has a relatively small U(eq) value). This difference is likely what triggered this alert.

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of C30 Check

**Author Response:** This atom assignment was confirmed as an oxygen (of a nitrate group). O9 is bonded directly to the Sm metal center (which has a relatively small U(eq) value). This difference is likely what triggered this alert.

PLAT242_ALERT_2_C Low	'MainMol' Ueq as Compared to Neighbors of	Sm1 Check
PLAT242_ALERT_2_C Low	'MainMol' Ueq as Compared to Neighbors of	N3 Check
PLAT242_ALERT_2_C Low	'MainMol' Ueq as Compared to Neighbors of	N4 Check
PLAT242_ALERT_2_C Low	'MainMol' Ueq as Compared to Neighbors of	C25 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including	O14	0.109 Check
PLAT331_ALERT_2_C Small Aver Phenyl C-C Dist C5	-C10	1.37 Ang.
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds .....		0.01919 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance .....		5.488 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=	0.600	91 Report
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..		1 Check
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.83A From O1		0.45 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.		0 Info

### Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...		6 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .....		4 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records		1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records		1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Sm1 --O5		5.6 s.u.
PLAT793_ALERT_4_G Model has Chirality at P2 (Centro SPGR)		R Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Sm1 (III)		3.46 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....		48 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=	0.600	125 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain

1 **ALERT level B** = A potentially serious problem, consider carefully

27 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
9 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
19 ALERT type 2 Indicator that the structure model may be wrong or deficient  
7 ALERT type 3 Indicator that the structure quality may be low  
9 ALERT type 4 Improvement, methodology, query or suggestion  
2 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.

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