

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SGGDC1

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: SGGDC1

Bond precision: C-C = 0.0114 A Wavelength=0.71073

Cell: a=16.9576(15) b=14.1250(11) c=19.769(2)
 alpha=90 beta=107.903(3) gamma=90

Temperature: 296 K

	Calculated	Reported
Volume	4505.9(7)	4505.9(7)
Space group	C 2/m	C 2/m
Hall group	-C 2y	-C 2y
Moiety formula	C31 H48 B Nb3 O S6, C H2 Cl2	?
Sum formula	C32 H50 B Cl2 Nb3 O S6	C32 H50 B Cl2 Nb3 O S6
Mr	1003.52	1003.52
Dx, g cm ⁻³	1.479	1.479
Z	4	4
Mu (mm ⁻¹)	1.170	1.170
F000	2032.0	2032.0
F000'	2011.21	
h, k, lmax	18, 15, 21	18, 15, 21
Nref	3141	3137
Tmin, Tmax	0.869, 0.911	0.740, 0.880
Tmin'	0.869	

Correction method= # Reported T Limits: Tmin=0.740 Tmax=0.880
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 22.618

R(reflections)= 0.0486(2005)

wR2(reflections)=
0.1084(3137)

S = 0.901

Npar= 244

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 A**

THETM01_ALERT_3_A The value of $\sin(\theta_{\max})/\lambda$ is less than 0.550
Calculated $\sin(\theta_{\max})/\lambda = 0.5411$

Author Response: Crystal was poorly diffracting at higher bragg angles.

PLAT601_ALERT_2_A Unit Cell Contains Solvent Accessible VOIDS of . 289 Ang**3

Author Response: Inspection of the final difference map shows that there are no significant left out peaks in the lattice. The voids may be typical to the geometry of molecule, inter molecular forces and resultant packing for minimum potential energy.

 **Alert level C**

PLAT260_ALERT_2_C Large Average Ueq of Residue Including C11	0.150	Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds	0.01144	Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance	12.322	Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance	2.178	Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.541	2	Report

 **Alert level G**

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite	19	Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...	28	Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records	3	Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records	1	Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records	6	Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records	1	Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used	0.0200	Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used	0.0200	Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used	0.0200	Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used	0.0200	Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used	0.0200	Report
PLAT300_ALERT_4_G Atom Site Occupancy of O1 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of C17 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16A Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16B Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16C Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17A Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17B Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17C Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of C11 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of C12 Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of C18 Constrained at	0.5	Check

PLAT300_ALERT_4_G	Atom Site Occupancy of H18A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H18B	Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)	5%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 2)	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in	(Resd 2)	2.50	Check
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond	C13 - C16	1.52	Ang.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		22.20	Deg.
	H16A -C16 -H16A	1_555 1_555 6_565	# 98	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		22.20	Deg.
	H16C -C16 -H16B	1_555 1_555 6_565	# 104	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		22.20	Deg.
	H16B -C16 -H16C	1_555 1_555 6_565	# 108	Check
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group	#	10	Check
PLAT822_ALERT_4_G	CIF-embedded .res Contains Negative PART Numbers		2	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		341	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary			Please Do !
PLAT899_ALERT_4_G	SHELXL2018 is Deprecated and Succeeded by SHELXL		2019/3	Note
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still		34%	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		2	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF		1	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		1	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		4.1	Low
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities			Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		0	Info

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

1 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
 17 ALERT type 3 Indicator that the structure quality may be low
 25 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* 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.

