checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mono

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.

Datablock: mono

Bond precision:	C-C = 0.0129 A		Wavelength=0.71073	
Cell:	a=9.1572(3)			
T	alpha=90 296 K	beta=102.87	27 (14)	gamma=90
Temperature:	290 K			
	Calculated		Reported	
Volume	2664.78(15)		2664.78(15))
Space group	C 2		C 2	
Hall group	C 2y		C 2y	
Moiety formula			C20 H30 Cl2	2 Nb2 O Se4
Sum formula		O Se4		2 Nb2 O Se4
Mr	859.00		859.00	
Dx,g cm-3	2.141		2.141	
Z	4		4	
, ,	6.535		6.535	
F000	1640.0		1640.0	
F000'	1623.40			
h,k,lmax	10,17,24		10,17,24	
	4702[2454]		4361	
<u>-</u>	0.254,0.375		0.303,0.44	1
Tmin'	0.200			
Correction method= # Reported T Limits: Tmin=0.303 Tmax=0.441 AbsCorr = MULTI-SCAN				
Data completeness= 1.78/0.93 Theta(max)= 24.998				
R(reflections) =	0.0301(3618)			wR2(reflections) = 0.0576(4361)
S = 0.861	Npar=	273		

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.

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Alert level C
PLAT241_ALERT_2_C High
                      'MainMol' Ueq as Compared to Neighbors of
                                                                         Sel Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of
                                                                         Se4 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of
                                                                         Nb2 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds .....
                                                                      0.0129 Ang.
  Alert level G
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem
                                                                         100 %Fit
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem
                                                                        100 %Fit
PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New Space Group
                                                                       Fdd2 Check
             Check Model Parameter Symmmetry for Reflection Data Support
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .
                                                                       1.14 Ratio
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .
                                                                     Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still
                                                                        60% Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ......
                                                                         3.9 Low
PLAT963_ALERT_2_G Both SHELXL WEIGHT Parameter Values Zero ......
                                                                     Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..
                                                                       50.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.
                                                                           0 Info
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   4 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  10 ALERT level G = General information/check it is not something unexpected
   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 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
   1 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 06/07/2023; check.def file version of 30/06/2023

