

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

Bond precision:	C-C = 0.0019 A	Wavelength=1.54184
Cell:	a=10.8226(1)	b=10.9399(2) c=17.3389(3)
	alpha=79.412(1)	beta=78.905(1) gamma=86.861(1)
Temperature:	100 K	
	Calculated	Reported
Volume	1979.82(5)	1979.82(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C13 H8 N2 O7 V, C6 H16 N	C13 H8 N2 O7 V, C6 H16 N
Sum formula	C19 H24 N3 O7 V	C19 H24 N3 O7 V
Mr	457.35	457.35
Dx,g cm-3	1.534	1.534
Z	4	4
Mu (mm-1)	4.621	4.621
F000	952.0	952.0
F000'	955.29	
h,k,lmax	12,13,20	12,13,20
Nref	7061	7061
Tmin,Tmax	0.397,0.747	0.621,1.000
Tmin'	0.286	

Correction method= # Reported T Limits: Tmin=0.621 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 1.000 Theta(max)= 67.078

R(reflections)= 0.0254(6958) wR2(reflections)= 0.0721(7061)

S = 1.061 Npar= 559

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 G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	8	Note
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.001	Degree
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	2	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) V1 --O3A .	5.2	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) V1 --O4A .	8.0	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) V1 --N1A .	7.0	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) V2 --O3B .	5.6	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) V2 --O4B .	7.2	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) V2 --N1B .	7.6	s.u.
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	4	Note
	C6 H16 N		
PLAT794_ALERT_5_G	Tentative Bond Valency for V1 (V) .	5.07	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for V2 (V) .	5.11	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	4	Note
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	97%	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged		Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	17	Info

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 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
2 ALERT type 4 Improvement, methodology, query or suggestion
2 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.

