

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelxl

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: shelxl

Bond precision: C-C = 0.0054 Å Wavelength=0.71073

Cell: a=10.4250 (3) b=14.3372 (5) c=16.9186 (6)
 alpha=70.239 (1) beta=88.969 (1) gamma=81.479 (1)
Temperature: 296 K

	Calculated	Reported
Volume	2352.16 (14)	2352.16 (14)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C21 H15 N3 O4 V, 2(O)	?
Sum formula	C21 H15 N3 O6 V	C21 H15 N3 O6 V
Mr	456.30	456.30
Dx, g cm ⁻³	1.288	1.289
Z	4	4
Mu (mm ⁻¹)	0.460	0.460
F000	932.0	932.0
F000'	933.64	
h, k, lmax	13, 19, 22	13, 19, 22
Nref	11823	11747
Tmin, Tmax	0.942, 0.946	0.943, 0.947
Tmin'	0.942	

Correction method= # Reported T Limits: Tmin=0.943 Tmax=0.947
AbsCorr = ?

Data completeness= 0.994 Theta(max)= 28.420

R(reflections)= 0.0590 (9365)	wR2(reflections)=
S = 1.074	0.2242 (11747)
Npar= 559	

test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

PLAT602_ALERT_2_A Solvent Accessible VOID(S) in Structure ! Check

PLAT230_ALERT_2_B	Hirshfeld Test Diff for C31	--C32	.	10.3	s.u.
PLAT260_ALERT_2_B	Large Average Ueq of Residue Including	O10		0.386	Check
PLAT260_ALERT_2_B	Large Average Ueq of Residue Including	O11		0.598	Check
PLAT260_ALERT_2_B	Large Average Ueq of Residue Including	O12		0.608	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)			09	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)			010	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)			011	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)			012	Check
PLAT430_ALERT_2_B	Short Inter D...A Contact O4	..O10	.	2.75	Ang.
		x,y,z =		1_555	Check
PLAT430_ALERT_2_B	Short Inter D...A Contact O4	..O9	.	2.83	Ang.
		x,y,z =		1_555	Check
PLAT934_ALERT_3_B	Number of (Iobs-Icalc)/Sigma(W) > 10	Outliers ..		8	Check

PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given	Please Do !
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C27	--C28 .	6.6 s.u.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C27	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C31	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C41	Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor		2.1 Note
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	O9	0.226 Check
PLAT430_ALERT_2_C	Short Inter D...A Contact O10	..O11 .	2.89 Ang.
	1-x,1-y,-z =		2_665 Check
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc)	.	14 Check
PLAT939_ALERT_3_C	Large Value of Not (SHELXL) Weight Optimized S	.	11.77 Check
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.49Ang From O10 .	0.84 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.83Ang From O12 .	0.43 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.88Ang From O12 .	-0.44 eA-3

PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	? Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.15 Report
PLAT093_ALERT_1_G	No s.u.'s on H-positions, Refinement Reported as	mixed Check
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.001 Degree
PLAT794_ALERT_5_G	Tentative Bond Valency for V1 (IV) .	4.21 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for V2 (IV) .	4.27 Info
PLAT899_ALERT_4_G	SHELXL-97 is Deprecated and Succeeded by SHELXL	2019/3 Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	3 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above Sth/L= 0.600	66 Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	1 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Densitv.	1 Info

1	ALERT level A	= Most likely a serious problem - resolve or explain
11	ALERT level B	= A potentially serious problem, consider carefully
13	ALERT level C	= Check. Ensure it is not caused by an omission or oversight
12	ALERT level G	= General information/check it is not something unexpected
4	ALERT type 1	CIF construction/syntax error, inconsistent or missing data
23	ALERT type 2	Indicator that the structure model may be wrong or deficient
5	ALERT type 3	Indicator that the structure quality may be low
2	ALERT type 4	Improvement, methodology, query or suggestion
3	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.

