

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1a, 1b, 2, 3

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: 1a

Bond precision:	C-C = 0.0036 Å	Wavelength=1.54184	
Cell:	a=16.4708(7)	b=16.8106(8)	c=7.5120(4)
	alpha=90	beta=90	gamma=90
Temperature:	150 K		
	Calculated	Reported	
Volume	2079.95(17)	2079.95(17)	
Space group	C c c 2	Ccc2	
Hall group	C 2 -2c	C 2 -2c	
Moiety formula	C20 H12 F6 O5 V	C20 H12 F6 O5 V	
Sum formula	C20 H12 F6 O5 V	C20 H12 F6 O5 V	
Mr	497.24	497.24	
Dx, g cm-3	1.588	1.588	
Z	4	4	
Mu (mm-1)	4.772	4.772	
F000	996.0	996.0	
F000'	1000.40		
h, k, lmax	20, 21, 9	20, 20, 9	
Nref	2146[1163]	1576	
Tmin, Tmax	0.892, 0.909	0.449, 0.911	
Tmin'	0.385		

Correction method= MULTI-SCAN

Data completeness= 1.36/0.73 Theta(max)= 74.730

R(reflections)= 0.0393(1357) wR2(reflections)= 0.1087(1576)

S = 1.059 Npar= 241

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

PLAT090_ALERT_3_B Poor Data / Parameter Ratio (Zmax > 18)	4.76	Note
PLAT915_ALERT_3_B Low Friedel Pair Coverage	44	%

🟢 Alert level C

PLAT213_ALERT_2_C Atom F1B	has ADP max/min Ratio	3.6	prolat
PLAT234_ALERT_4_C Large Hirshfeld Difference C8A	-- C9A ..	0.18	Ang.
PLAT242_ALERT_2_C Low	Ueq as Compared to Neighbors for	C6	Check
PLAT332_ALERT_2_C Large Phenyl C-C Range	C5 -C10A	0.20	Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact H3	.. H10A ..	1.99	Ang.
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=	0.600	2	Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF		1	Note

🟠 Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite		18	Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...		8	Report
PLAT004_ALERT_5_G Polymeric Structure Found with Dimension		1	Info
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF			Please Do !
PLAT242_ALERT_2_G Low	Ueq as Compared to Neighbors for	C1	Check
PLAT301_ALERT_3_G Main Residue Disorder	Percentage =	62	Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .		1.18	Ratio
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms			! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints		69	Note
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL		2014	Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=	0.600	14	Note

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

0 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
6 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

Datablock: 1b

Bond precision:	C-C = 0.0050 A	Wavelength=0.71073	
Cell:	a=16.7507(10)	b=16.8587(14)	c=7.5561(6)
	alpha=90	beta=90	gamma=90
Temperature:	293 K		

	Calculated	Reported
Volume	2133.8(3)	2133.8(3)
Space group	C c c 2	Ccc2
Hall group	C 2 -2c	C 2 -2c
Moiety formula	C20 H12 F6 O5 V	C20 H12 F6 O5 V
Sum formula	C20 H12 F6 O5 V	C20 H12 F6 O5 V
Mr	497.24	497.24
Dx, g cm-3	1.548	1.548
Z	4	4
Mu (mm-1)	0.545	0.545
F000	996.0	996.0
F000'	997.98	
h, k, lmax	21, 21, 9	21, 21, 9
Nref	2449[1323]	1929
Tmin, Tmax	0.968, 0.973	0.876, 0.973
Tmin'	0.873	

Correction method= MULTI-SCAN

Data completeness= 1.46/0.79 Theta(max)= 27.470

R(reflections)= 0.0533(1340) wR2(reflections)= 0.1295(1929)

S = 1.104 Npar= 234

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

PLAT090_ALERT_3_B Poor Data / Parameter Ratio (Zmax > 18) 5.56 Note

Alert level C

PLAT213_ALERT_2_C Atom F2A	has ADP max/min Ratio	3.3 prolat
PLAT213_ALERT_2_C Atom F1B	has ADP max/min Ratio	3.1 prolat
PLAT234_ALERT_4_C Large Hirshfeld Difference F1B	-- C1 ..	0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F2B	-- C1 ..	0.20 Ang.
PLAT331_ALERT_2_C Small Average Phenyl C-C Dist. C5	-C10A	1.37 Ang.
PLAT332_ALERT_2_C Large Phenyl C-C Range C5	-C10B	0.24 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance		6.339 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600		18 Report
PLAT915_ALERT_3_C Low Friedel Pair Coverage		56 %

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite		7 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...		2 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Dimension		1 Info
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF		Please Do !
PLAT199_ALERT_1_G Reported _cell_measurement_temperature	(K)	293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature	(K)	293 Check

PLAT242_ALERT_2_G	Low Ueq as Compared to Neighbors for	C1 Check
PLAT301_ALERT_3_G	Main Residue Disorder Percentage =	62 Note
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.18 Ratio
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	! Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	38 Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2014 Note
PLAT910_ALERT_3_G	Missing # of FCF Reflections Below Th(Min)	3 Report

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Datablock: 2

Bond precision: C-C = 0.0039 A

Wavelength=0.71073

Cell: a=7.5066(3) b=10.6366(6) c=10.7430(5)
 alpha=88.063(3) beta=75.206(3) gamma=85.574(3)

Temperature: 293 K

	Calculated	Reported
Volume	826.78(7)	826.78(7)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C10 H14 O5 V, C5 H5 N O	C10 H14 O5 V, C5 H5 N O
Sum formula	C15 H19 N O6 V	C15 H19 N O6 V
Mr	360.25	360.25
Dx, g cm-3	1.447	1.447
Z	2	2
Mu (mm-1)	0.629	0.629
F000	374.0	374.0
F000'	374.79	
h, k, lmax	9, 13, 13	9, 13, 13
Nref	3779	3673
Tmin, Tmax	0.927, 0.951	0.885, 0.951
Tmin'	0.882	

Correction method= MULTI-SCAN

Data completeness= 0.972

Theta(max)= 27.440

R(reflections)= 0.0472(2915) wR2(reflections)= 0.1340(3673)

S = 1.077 Npar= 212

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

PLAT910_ALERT_3_A Missing # of FCF Reflections Below Th(Min) 83 Report

 Alert level B

PLAT430_ALERT_2_B Short Inter D...A Contact 03 .. 06 .. 2.77 Ang.

 Alert level C

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low 0.972 Note
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 5 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF 4 Note

 Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 1 Report
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal 0.00300 Degree
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 18 Note

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- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
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Datablock: 3

Bond precision: C-C = 0.0042 A Wavelength=0.71073

Cell: a=10.5709(3) b=9.9246(4) c=13.4691(4)
 alpha=90 beta=115.553(2) gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	1274.85(8)	1274.85(7)
Space group	P 21/c	P21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C6 H4 Cl N O4 V, C5 H6 N	C6 H4 Cl N O4 V, C5 H6 N
Sum formula	C11 H10 Cl N2 O4 V	C11 H10 Cl N2 O4 V
Mr	320.60	320.60
Dx, g cm-3	1.670	1.670
Z	4	4
Mu (mm-1)	0.998	0.998
F000	648.0	648.0
F000'	650.06	
h, k, lmax	13, 12, 17	13, 12, 17
Nref	2915	2893
Tmin, Tmax	0.920, 0.951	0.825, 0.952
Tmin'	0.819	

Correction method= MULTI-SCAN

Data completeness= 0.992

Theta(max)= 27.460

R(reflections)= 0.0375(2230)

wR2(reflections)= 0.1047(2893)

S = 1.042

Npar= 174

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 C

PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600

19 Report



Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF

Please Do !

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms

1 Report

PLAT128_ALERT_4_G Alternate Setting for Input Space Group P21/c

P21/n Note

PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K)

293 Check

PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K)

293 Check

PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL

2014 Note

PLAT910_ALERT_3_G Missing # of FCF Reflections Below Th(Min)

4 Report

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

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1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

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2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

0 ALERT type 2 Indicator that the structure model may be wrong or deficient

2 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

checkCIF publication errors

Alert level A

PUBL012_ALERT_1_A _publ_section_abstract is missing.
Abstract of paper in English.

Alert level G

PUBL017_ALERT_1_G The _publ_section_references section is missing or empty.

-
- 1 **ALERT level A** = Data missing that is essential or data in wrong format
 - 1 **ALERT level G** = General alerts. Data that may be required is missing
-

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
_vrf_PLAT910_2
;
PROBLEM: Missing # of FCF Reflections Below Th(Min) .....      83 Report
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 20/08/2014; check.def file version of 18/08/2014

Datablock 1a - ellipsoid plot







