

# 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

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Bond precision:    C-C = 0.0073 Å                      Wavelength=0.71073

Cell:                      a=20.040(4)              b=26.118(5)              c=36.745(11)  
                            alpha=90              beta=90              gamma=90  
Temperature:              150 K

	Calculated	Reported
Volume	19233(8)	19232(8)
Space group	F d d d	F d d d
Hall group	: -F 2uv 2v	-F 2uv 2v
	C32 H34 K2 N4 O17 Ti2, C	
Moiety formula	H3 O, C O2, 2(C0.50 O0.50), 2(C0.50 O0	C36 H37 K2 N4 O22 Ti2
Sum formula	C36 H37 K2 N4 O22 Ti2	C36 H37 K2 N4 O22 Ti2
Mr	1051.64	1051.69
Dx, g cm <sup>-3</sup>	1.453	1.453
Z	16	16
Mu (mm <sup>-1</sup> )	0.587	0.587
F000	8624.0	8624.0
F000'	8644.21	
h,k,lmax	25,32,46	25,32,45
Nref	5004	4976
Tmin,Tmax	0.889,0.943	0.658,0.745
Tmin'	0.889	

Correction method= # Reported T Limits: Tmin=0.658 Tmax=0.745  
AbsCorr = EMPIRICAL

Data completeness= 0.994                      Theta(max)= 26.515

R(reflections)= 0.0718( 3261)              wR2(reflections)= 0.2215( 4976)

S = 1.052                      Npar= 304

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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

PLAT413_ALERT_2_B	Short Inter XH3 .. XHn	H3	..H97C	.	1.97 Ang.
			x,y,z =		1_555 Check
PLAT430_ALERT_2_B	Short Inter D...A Contact	O12	..O98B	.	2.61 Ang.
			x,y,z =		1_555 Check
PLAT430_ALERT_2_B	Short Inter D...A Contact	O17	..O98A	.	2.72 Ang.
			1/2-x,-y,3/2-z =		25_556 Check
PLAT430_ALERT_2_B	Short Inter D...A Contact	O17	..O98B	.	2.74 Ang.
			1/2-x,-y,3/2-z =		25_556 Check
PLAT780_ALERT_1_B	Coordinates do not Form a Properly Connected Set				Please Do !

### Alert level C

RINTA01_ALERT_3_C	The value of Rint is greater than 0.12				
	Rint given	0.123			
PLAT020_ALERT_3_C	The Value of Rint is Greater Than 0.12	.....	0.123	Report	
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	O97	0.123	Check	
PLAT309_ALERT_2_C	Single Bonded Oxygen (C-O > 1.3 Ang)	.....	O97	Check	
PLAT309_ALERT_2_C	Single Bonded Oxygen (C-O > 1.3 Ang)	.....	O17	Check	
PLAT309_ALERT_2_C	Single Bonded Oxygen (C-O > 1.3 Ang)	.....	O98A	Check	
PLAT309_ALERT_2_C	Single Bonded Oxygen (C-O > 1.3 Ang)	.....	O98B	Check	
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	.....	0.00729	Ang.	
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	.....	2.122	Check	
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.		0	Info	

### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		7	Note	
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		3	Info	
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	.....	3	Report	
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ		Please	Check	
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large		231.38	Why ?	
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records		5	Report	
PLAT300_ALERT_4_G	Atom Site Occupancy of C97	Constrained at	0.5	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of H97A	Constrained at	0.5	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of H97B	Constrained at	0.5	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of H97C	Constrained at	0.5	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of C17B	Constrained at	0.5	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of O98A	Constrained at	0.5	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of C98A	Constrained at	0.5	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of O98B	Constrained at	0.5	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of C98B	Constrained at	0.5	Check	
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2 )		50%	Note	
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3 )		33%	Note	
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4 )		100%	Note	
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5 )		100%	Note	
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O17 ..C97	2.90	Ang.	
		-1/2+x,1/4-y,7/4-z =	11_456	Check	
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O98A ..C98B	2.00	Ang.	
		1/2-x,-y,3/2-z =	25_556	Check	
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O98A ..C17B	2.06	Ang.	
		1/2-x,-y,3/2-z =	25_556	Check	
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O98B ..C17B	1.49	Ang.	
		1/2-x,-y,3/2-z =	25_556	Check	
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O98B ..C98A	2.38	Ang.	
		1/2-x,-y,3/2-z =	25_556	Check	

PLAT432_ALERT_2_G Short Inter X...Y Contact	C17B ..C98B	2.32 Ang.
	1/2-x,-y,3/2-z =	25_556 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C17B ..C98A	3.09 Ang.
	x,y,z =	1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C17B ..C98A	3.19 Ang.
	1/2-x,-y,3/2-z =	25_556 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C97 ..C97	2.54 Ang.
	7/4-x,3/4-y,z =	14_655 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C97 ..C97	2.84 Ang.
	x,3/4-y,7/4-z =	7_556 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C98A ..C98B	0.97 Ang.
	1/2-x,-y,3/2-z =	25_556 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .		1.16 Ratio
PLAT794_ALERT_5_G Tentative Bond Valency for Ti1 (IV) .		4.17 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....		5 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=	0.600	26 Note

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

2 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  
 16 ALERT type 4 Improvement, methodology, query or suggestion  
 3 ALERT type 5 Informative message, check

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## 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_RINTA01_shelx
;
PROBLEM: The value of Rint is greater than 0.12
RESPONSE: ...
;
_vrf_PLAT020_shelx
;
PROBLEM: The Value of Rint is Greater Than 0.12 ..... 0.123 Report
RESPONSE: ...
;
_vrf_PLAT260_shelx
;
PROBLEM: Large Average Ueq of Residue Including 097 0.123 Check
RESPONSE: ...
;
_vrf_PLAT309_shelx
;
PROBLEM: Single Bonded Oxygen (C-O > 1.3 Ang) ..... 097 Check
RESPONSE: ...
;
_vrf_PLAT341_shelx
;
PROBLEM: Low Bond Precision on C-C Bonds ..... 0.00729 Ang.
RESPONSE: ...
;
_vrf_PLAT906_shelx
```

```
;
PROBLEM: Large K Value in the Analysis of Variance ..... 2.122 Check
RESPONSE: ...
;
_vrf_PLAT978_shelx
;
PROBLEM: Number C-C Bonds with Positive Residual Density. 0 Info
RESPONSE: ...
;
# end Validation Reply Form
```

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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.

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**PLATON version of 19/10/2018; check.def file version of 15/10/2018**

