

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) k

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: k

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Bond precision:	C-C = 0.0113 Å	Wavelength=1.34050
Cell:	a=11.0912 (8)	b=22.8365 (14)      c=22.7541 (13)
	alpha=90	beta=90.580 (6)      gamma=90
Temperature:	293 K	
	Calculated	Reported
Volume	5763.0 (6)	5763.0 (6)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C48 H47 N6 O16 Ti3, C2 H3 N, H2 O	C48 H47 N6 O16 Ti3, C2 H3 N, H2 O
Sum formula	C50 H52 N7 O17 Ti3	C50 H52 N7 O17 Ti3
Mr	1166.60	1166.68
Dx, g cm <sup>-3</sup>	1.345	1.345
Z	4	4
Mu (mm <sup>-1</sup> )	2.743	2.743
F000	2412.0	2412.0
F000'	2421.76	
h, k, lmax	13, 27, 27	13, 26, 27
Nref	10302	9873
Tmin, Tmax	0.735, 0.740	
Tmin'	0.667	

Correction method= Not given

Data completeness= 0.958

Theta (max)= 53.221

R(reflections)= 0.0796 ( 7245)

wR2(reflections)=  
0.2441 ( 9873)

S = 1.025

Npar= 697

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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.

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### Alert level B

PLAT029_ALERT_3_B	_diffn_measured_fraction_theta_full	value	Low	.	0.958	Why?
PLAT220_ALERT_2_B	NonSolvent	Resd 1	C	Ueq(max)/Ueq(min)	Range	7.9 Ratio
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	C01Z	--C024	.	8.0	s.u.
PLAT234_ALERT_4_B	Large Hirshfeld Difference	O00I	--C01Z	.	0.28	Ang.
PLAT234_ALERT_4_B	Large Hirshfeld Difference	C01T	--C021	.	0.28	Ang.
PLAT241_ALERT_2_B	High	'MainMol'	Ueq as Compared to Neighbors of		C01Z	Check
PLAT242_ALERT_2_B	Low	'MainMol'	Ueq as Compared to Neighbors of		O00I	Check
PLAT315_ALERT_2_B	Singly Bonded Carbon Detected	(H-atoms Missing).			C022	Check
PLAT360_ALERT_2_B	Short	C(sp3)-C(sp3) Bond	C01Z	- C024	.	1.28 Ang.
PLAT412_ALERT_2_B	Short	Intra XH3 .. XHn	H01T	..H02C	.	1.78 Ang.
				x,y,z =	1_555	Check
PLAT417_ALERT_2_B	Short	Inter D-H..H-D	H01I	..H1WA	.	2.08 Ang.
				x,y,z =	1_555	Check
PLAT417_ALERT_2_B	Short	Inter D-H..H-D	H01K	..H1WB	.	1.91 Ang.
				1-x,-1/2+y,1/2-z =	2_645	Check

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### Alert level C

RADNW01_ALERT_1_C	The radiation wavelength lies outside the expected range					
	for the supplied radiation type. Expected range	1.34130-1.34150				
	Wavelength given =	1.34050				
PLAT031_ALERT_4_C	Refined Extinction Parameter Within Range	.....			3.111	Sigma
PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given			Please	Do !
PLAT202_ALERT_3_C	Isotropic non-H Atoms in Anion/Solvent	.....			1	Check
	O1W					
PLAT213_ALERT_2_C	Atom C01Z	has ADP max/min Ratio	.....		4.0	prolat
PLAT222_ALERT_3_C	NonSolvent	Resd 1	H	Uiso(max)/Uiso(min)	Range	8.4 Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C01X	--C020	.	5.2	s.u.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C01T	--C022	.	0.18	Ang.
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of		O00E	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of		C01F	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of		C01I	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of		C01R	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of		C01T	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of		C01X	Check
PLAT244_ALERT_4_C	Low	'Solvent'	Ueq as Compared to Neighbors of		C01O	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	Ti01			0.103	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	N01P			0.149	Check
PLAT334_ALERT_2_C	Small Aver. Benzene C-C Dist	C00O	-C018		1.37	Ang.
PLAT341_ALERT_3_C	Low Bond Precision on	C-C Bonds	.....		0.01126	Ang.
PLAT360_ALERT_2_C	Short	C(sp3)-C(sp3) Bond	C01T	- C021	.	1.36 Ang.
PLAT360_ALERT_2_C	Short	C(sp3)-C(sp3) Bond	C01Z	- C023	.	1.36 Ang.
PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N01H	--H01H	.	Please	Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N01H	--H01I	.	Please	Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N01K	--H01K	.	Please	Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N01U	--H01P	.	Please	Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N01Y	--H01U	.	Please	Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N01Y	--H01W	.	Please	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	.....			8.649	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	.....			2.397	Check

PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.598	420	Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .		1	Check
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.93A From O1W		-0.52	eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.66A From O1W		-0.49	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H1WA		-0.51	eA-3



### Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu not performed for this radiation type.				
PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		2	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...		6	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....		14	Report
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large		0.14	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large		6.60	Why ?
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records		1	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records		6	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature ..... (K)		293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature ..... (K)		293	Check
PLAT343_ALERT_2_G	Unusual sp3 Angle Range in Main Residue for		C01T	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for		C022	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....		127	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # C2 H3 N		2	Note
PLAT793_ALERT_4_G	Model has Chirality at C01T (Centro SPGR)		R	Verify
PLAT794_ALERT_5_G	Tentative Bond Valency for TiO2 (IV) .		4.27	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....		37	Note
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		40%	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....		3.2	Low
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  
 12 **ALERT level B** = A potentially serious problem, consider carefully  
 34 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 21 **ALERT level G** = General information/check it is not something unexpected

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 38 ALERT type 2 Indicator that the structure model may be wrong or deficient  
 11 ALERT type 3 Indicator that the structure quality may be low  
 10 ALERT type 4 Improvement, methodology, query or suggestion  
 2 ALERT type 5 Informative message, check

## 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_RADNW01_k
;
PROBLEM: The radiation wavelength lies outside the expected range
RESPONSE: ...
;
_vrf_PLAT031_k
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;
PROBLEM: Refined Extinction Parameter Within Range ..... 3.111 Sigma
RESPONSE: ...
;
_vrf_PLAT052_k
;
PROBLEM: Info on Absorption Correction Method Not Given Please Do !
RESPONSE: ...
;
_vrf_PLAT202_k
;
PROBLEM: Isotropic non-H Atoms in Anion/Solvent ..... 1 Check
RESPONSE: ...
;
_vrf_PLAT213_k
;
PROBLEM: Atom C01Z has ADP max/min Ratio ..... 4.0 prolat
RESPONSE: ...
;
_vrf_PLAT222_k
;
PROBLEM: NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 8.4 Ratio
RESPONSE: ...
;
_vrf_PLAT230_k
;
PROBLEM: Hirshfeld Test Diff for C01X --C020 . 5.2 s.u.
RESPONSE: ...
;
_vrf_PLAT234_k
;
PROBLEM: Large Hirshfeld Difference C01T --C022 . 0.18 Ang.
RESPONSE: ...
;
_vrf_PLAT242_k
;
PROBLEM: Low 'MainMol' Ueq as Compared to Neighbors of 000E Check
RESPONSE: ...
;
_vrf_PLAT244_k
;
PROBLEM: Low 'Solvent' Ueq as Compared to Neighbors of C010 Check
RESPONSE: ...
;
_vrf_PLAT260_k
;
PROBLEM: Large Average Ueq of Residue Including Ti01 0.103 Check
RESPONSE: ...
;
_vrf_PLAT334_k
;
PROBLEM: Small Aver. Benzene C-C Dist C000 -C018 1.37 Ang.
RESPONSE: ...
;
_vrf_PLAT341_k
;
PROBLEM: Low Bond Precision on C-C Bonds ..... 0.01126 Ang.

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RESPONSE: ...
;
_vrf_PLAT360_k
;
PROBLEM: Short C(sp3)-C(sp3) Bond C01T - C021 . 1.36 Ang.
RESPONSE: ...
;
_vrf_PLAT420_k
;
PROBLEM: D-H Bond Without Acceptor N01H --H01H . Please Check
RESPONSE: ...
;
_vrf_PLAT906_k
;
PROBLEM: Large K Value in the Analysis of Variance ..... 8.649 Check
RESPONSE: ...
;
_vrf_PLAT911_k
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L= 0.598 420 Report
RESPONSE: ...
;
_vrf_PLAT918_k
;
PROBLEM: Reflection(s) with I(obs) much Smaller I(calc) . 1 Check
RESPONSE: ...
;
_vrf_PLAT976_k
;
PROBLEM: Check Calcd Resid. Dens. 0.93A From O1W -0.52 eA-3
RESPONSE: ...
;
_vrf_PLAT977_k
;
PROBLEM: Check Negative Difference Density on H1WA -0.51 eA-3
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.

