

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I

Bond precision:	C-C = 0.0059 A	Wavelength=0.71073
Cell:	a=15.1689(6)	b=15.1689(6) c=15.1689(6)
	alpha=90	beta=90 gamma=90
Temperature:	295 K	
	Calculated	Reported
Volume	3490.3(4)	3490.3(4)
Space group	P 21 3	P 21 3
Hall group	P 2ac 2ab 3	?
Moiety formula	C21 H30 O18 Ti, 2(H4 N), 2(H2 O)	C21 H41.99 N2.00 O20.00 Ti1.00
Sum formula	C21 H41.99 N2 O20 Ti	C21 H41.99 N2.00 O20.00 Ti1.00
Mr	690.32	690.35
Dx, g cm ⁻³	1.314	1.314
Z	4	4
Mu (mm ⁻¹)	0.323	0.323
F000	1455.7	1455.7
F000'	1457.85	
h, k, lmax	18, 18, 18	12, 13, 18
Nref	2382[1326]	2392
Tmin, Tmax	0.940, 0.965	0.950, 0.970
Tmin'	0.940	

Correction method= # Reported T Limits: Tmin=0.950 Tmax=0.970

AbsCorr = NUMERICAL

Data completeness= 1.80/1.00

Theta(max)= 26.391

R(reflections)= 0.0531(1927)

wR2(reflections)=
0.1492(1927)

S = 1.000

Npar= 151

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

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT076_ALERT_1_C	Occupancy 0.333 Less Than 1.0 for Sp.pos .	N2
PLAT076_ALERT_1_C	Occupancy 0.333 Less Than 1.0 for Sp.pos .	H21
PLAT420_ALERT_2_C	D-H Bond Without Acceptor N1 --H13 .	Please Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	8 Report



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	6 Note
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	17 Report
PLAT093_ALERT_1_G	No s.u.'s on H-positions, Refinement Reported as	mixed Check
PLAT300_ALERT_4_G	Atom Site Occupancy of T11 Constrained at	0.999 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N1 Constrained at	0.666 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13 Constrained at	0.666 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H14 Constrained at	0.666 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N2 Constrained at	0.333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H21 Constrained at	0.333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H24 Constrained at	0.333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O7 Constrained at	0.2 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H71 Constrained at	0.2 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H72 Constrained at	0.2 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O8 Constrained at	0.2 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H81 Constrained at	0.2 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H82 Constrained at	0.2 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O9 Constrained at	0.266 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H91 Constrained at	0.266 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H92 Constrained at	0.266 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N3 Constrained at	0.333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H31 Constrained at	0.333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H32 Constrained at	0.333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H33 Constrained at	0.333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H34 Constrained at	0.333 Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	7% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100% 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
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 6)	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 7)	100% Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 2)	3.33 Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 3)	1.66 Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 4)	0.60 Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 5)	0.60 Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 6)	0.80 Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 7)	1.66 Check

PLAT769_ALERT_4_G	CIF Embedded explicitly supplied scattering data	Please Note
PLAT791_ALERT_4_G	Model has Chirality at C4 (Sohnke SpGr)	R Verify
PLAT791_ALERT_4_G	Model has Chirality at C6 (Sohnke SpGr)	R Verify
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found	Please Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	7 Note
PLAT882_ALERT_1_G	No Datum for _diffrn_reflms_av_unetI/netI	Please Do !
PLAT929_ALERT_5_G	No Weight Pars,Obs and Calc R1,wR2,S not Checked	! Info
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...	9 Check

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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
36 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.

