

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Ti2-Phen

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: Ti2-Phen

Bond precision:	C-C = 0.0033 A	Wavelength=1.54178
Cell:	a=45.092 (12) b=19.851 (6) c=30.826 (8)	alpha=90 beta=130.034 (10) gamma=90
Temperature:	173 K	
	Calculated	Reported
Volume	21127 (11)	21126 (10)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	2(C112 H120 N4 O8 Ti2), C3 H8 O [+ solvent]	2(C112 H120 N4 O8 Ti2), C3 H8 O
Sum formula	C227 H248 N8 O17 Ti4 [+ solvent]	C227 H248 N8 O17 Ti4
Mr	3551.81	3551.92
Dx, g cm ⁻³	1.117	1.117
Z	4	4
Mu (mm ⁻¹)	1.718	1.718
F000	7560.0	7560.0
F000'	7583.35	
h, k, lmax	53, 23, 36	53, 23, 36
Nref	18881	18826
Tmin, Tmax	0.806, 0.996	0.617, 0.754
Tmin'	0.806	

Correction method= # Reported T Limits: Tmin=0.617 Tmax=0.754
AbsCorr = MULTI-SCAN

Data completeness= 0.997

Theta(max)= 67.075

R(reflections) = 0.0420(16242)

wR2(reflections) =
0.1211(18826)

S = 1.063

Npar = 1415

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

PLAT220_ALERT_2_C	NonSolvent	Resd 1	C	Ueq(max)/Ueq(min) Range	5.5 Ratio
PLAT221_ALERT_2_C	Solv./Anion	Resd 2	C	Ueq(max)/Ueq(min) Range	4.8 Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 1	H	Uiso(max)/Uiso(min) Range	6.0 Ratio
PLAT223_ALERT_4_C	Solv./Anion	Resd 2	H	Ueq(max)/Ueq(min) Range	5.0 Ratio
PLAT242_ALERT_2_C	Low	'MainMol'		Ueq as Compared to Neighbors of	C90 Check
PLAT242_ALERT_2_C	Low	'MainMol'		Ueq as Compared to Neighbors of	C49 Check
PLAT242_ALERT_2_C	Low	'MainMol'		Ueq as Compared to Neighbors of	C51 Check
PLAT242_ALERT_2_C	Low	'MainMol'		Ueq as Compared to Neighbors of	C76 Check
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. #				1 Note
		C112 H120 N4 O8 Ti2			
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.597			48 Report
	1 23 0, 3 1 0, 6 2 0, -16 2 1, -4 4 1, -3 1 1,				
	-1 23 1, 1 1 1, 1 23 1, 3 23 1, 9 23 1, -4 0 2,				
	-1 1 2, 0 0 2, 2 0 2, 3 3 2, 5 1 2, -5 3 3,				
	-2 4 3, 0 2 3, -8 0 4, -6 0 4, -6 4 4, 0 2 4,				
	-4 0 6, -12 0 8, -18 4 9, -18 4 10, -13 5 11, -18 4 12,				
	12 0 12, -20 0 16, -29 19 19, -28 18 22, -24 2 23, -28 16 25,				
	-25 1 25, -26 0 26, -27 15 27, -30 0 28, -28 14 28, -26 0 28,				
	-27 13 30, -47 1 34, -46 0 34, -44 0 34, -45 1 35, -42 0 36,				
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF				8 Note
	1 1 0, -1 1 1, -4 0 2, 2 0 2, 3 3 2, -8 0 4,				
	-6 0 4, -6 4 4,				

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	47 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	91 Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1 Report
	H2	
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	13.68 Why ?
PLAT128_ALERT_4_G	Alternate Setting for Input Space Group C2/c	I2/a Note
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	19 Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	8 Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0040 Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0040 Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0040 Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0040 Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0040 Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0040 Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0020 Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0020 Report
PLAT300_ALERT_4_G	Atom Site Occupancy of O2	Constrained at 0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C38	Constrained at 0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C100	Constrained at 0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C102	Constrained at 0.5 Check

PLAT300_ALERT_4_G	Atom Site Occupancy of H2	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H10J	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H10K	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H10L	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H38A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H38B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H38C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H100	Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)	19%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 2)	14%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 3)	100%	Note
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn	H3AA ..H103	.	2.14 Ang.
		x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn	H32 ..H6AB	.	1.96 Ang.
		x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn	H47 ..H4AB	.	2.07 Ang.
		x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn	H83 ..H94B	.	2.07 Ang.
		x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn	H85 ..H12A	.	1.98 Ang.
		x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn	H93 ..H21C	.	2.11 Ang.
		x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn	H15B ..H29	.	2.10 Ang.
		x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn	H29 ..H15E	.	2.01 Ang.
		x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn	H36 ..H10G	.	1.98 Ang.
		x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn	H63 ..H8C	.	2.11 Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O2 ..C48	.	2.71 Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O2 ..C107	.	3.01 Ang.
		1-x,-1+y,1/2-z =	2_645	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C25 ..C60	.	3.20 Ang.
		1-x,y,1/2-z =	2_655	Check
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure		167	A**3
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		27	Note
	H9AA H9AB H9AC H7AA H7AB H7AC H8AA H8AB			
	H8AC H1AA H1AB H1AC H2AA H2AB H2AC H3AA			
	H3AB H3AC H5AA H5AB H5AC H4AA H4AB H4AC			
	H6AA H6AB H6AC			
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C57	--C5A	1.71	Ang.
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #		12	Check
PLAT822_ALERT_4_G	CIF-embedded .res Contains Negative PART Numbers		3	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		809	Note
PLAT868_ALERT_4_G	ALERTS Due to the Use of _smtbx_masks Suppressed		!	Info
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		74%	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		3	Note
	1 1 0, 2 0 0, -1 1 1,			
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		1	Note
	-26 0 26,			
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		4.6	Low
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value		3.55	Note
	Predicted wR2: Based on SigI**2	3.41 or SHELX Weight	11.84	

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
25 ALERT type 2 Indicator that the structure model may be wrong or deficient
16 ALERT type 3 Indicator that the structure quality may be low
24 ALERT type 4 Improvement, methodology, query or suggestion
2 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.

