

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 9

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: 9

Bond precision: C-C = 0.0068 A Wavelength=0.71073

Cell: a=21.5207(11) b=13.1782(5) c=18.0083(14)
 alpha=90 beta=110.869(8) gamma=90

Temperature: 150 K

	Calculated	Reported
Volume	4772.2(5)	4772.2(5)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C36 H88 N3 Si6 Th	C36 H88 N3 Si6 Th
Sum formula	C36 H88 N3 Si6 Th	C36 H88 N3 Si6 Th
Mr	963.67	963.67
Dx,g cm-3	1.341	1.341
Z	4	4
Mu (mm-1)	3.301	3.301
F000	1996.0	1996.0
F000'	1969.54	
h,k,lmax	25,15,21	25,15,21
Nref	4365	4339
Tmin,Tmax	0.751,0.841	0.935,1.000
Tmin'	0.247	

Correction method= # Reported T Limits: Tmin=0.935 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.994 Theta(max)= 25.349

R(reflections)= 0.0395(3598) wR2(reflections)= 0.0751(4339)

S = 1.110 Npar= 237

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**

PLAT324_ALERT_2_C	Check for Possibly Missing H on Coordinating...	N1	Check
PLAT324_ALERT_2_C	Check for Possibly Missing H on Coordinating...	N2	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	3.312	Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).	8	Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	18	Report
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.	0	Info

● **Alert level G**

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	25	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	1	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Th1 --Si1 .	8.8	s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of Th1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of ClA Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1AA Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1B Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1AB Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1AC Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H14A Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	7%	Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	3	Note
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #	10	Check
	N1 -Si1 -Th1 1.555 1.555 2.655	39.46	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #	20	Check
	ClA -Si1 -Cl 1.555 1.555 1.555	14.10	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #	23	Check
	N1 -Si2 -Th1 1.555 1.555 2.655	39.07	Deg.
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #	8	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	212	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	2	Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
6 **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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 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
16 ALERT type 4 Improvement, methodology, query or suggestion
0 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.

PLATON version of 09/11/2017; check.def file version of 08/11/2017

