

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: naka381

Bond precision:	C-C = 0.0030 A	Wavelength=0.71073	
Cell:	a=9.3227 (7)	b=27.786 (2)	c=11.5041 (9)
	alpha=90	beta=94.503 (1)	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	2970.8 (4)	2970.9 (4)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C24 H28 Cl Fe N2 O4 P Si, C4 H8 O	C24 H28 Cl Fe N2 O4 P Si, C4 H8 O	
Sum formula	C28 H36 Cl Fe N2 O5 P Si	C28 H36 Cl Fe N2 O5 P Si	
Mr	630.95	630.95	
Dx, g cm ⁻³	1.411	1.411	
Z	4	4	
Mu (mm ⁻¹)	0.732	0.732	
F000	1320.0	1320.0	
F000'	1323.15		
h, k, lmax	11, 33, 13	11, 33, 13	
Nref	5536	5528	
Tmin, Tmax	0.851, 0.877	0.856, 0.880	
Tmin'	0.851		
Correction method=	# Reported T Limits: Tmin=0.856 Tmax=0.880		
AbsCorr =	NUMERICAL		
Data completeness=	0.999	Theta(max)= 25.497	
R(reflections)=	0.0296 (4670)	wR2(reflections)=	0.0767 (5528)
S =	1.021	Npar=	404

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 G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	10	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	10	Report
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	?	Check
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	20	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	2	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	2	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	2	Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for O1 --C21 .	6.2	s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for O2 --C22 .	6.2	s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for O3 --C23 .	6.6	s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for O4 --C24 .	7.9	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Fe1 --C21 .	10.2	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Fe1 --C22 .	10.1	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Fe1 --C23 .	9.9	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Fe1 --C24 .	10.1	s.u.
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
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 2)	9.39	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 3)	3.61	Check
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O5 .	101.7	Degree
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	40.12	Deg.
	N1 -SI1 -P1 1_555 1_555 1_555 #	17	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	40.22	Deg.
	N2 -SI1 -P1 1_555 1_555 1_555 #	18	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	44.95	Deg.
	N1 -P1 -SI1 1_555 1_555 1_555 #	27	Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	2	Note
	C4 H8 O		
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	3	Note
	C4 H8 O		
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	160	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please	Do !
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	2	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.6	Low
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	51.0	Degree

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

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

