

R(reflections)= 0.0338( 2825)	wR2(reflections)= 0.0873( 3239)
S = 1.053	Npar= 220

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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 A

PLAT971_ALERT_2_A	Check Calcd Resid. Dens. 1.03Ang From C1S	5.11 eA-3
PLAT973_ALERT_2_A	Check Calcd Positive Resid. Density on Ir1	2.53 eA-3

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#### Alert level B

PLAT094_ALERT_2_B	Ratio of Maximum / Minimum Residual Density ....	4.71 Report
PLAT196_ALERT_1_B	No TEMP record and _measurement_temperature .NE.	293 Degree
PLAT971_ALERT_2_B	Check Calcd Resid. Dens. 0.77Ang From C11S	2.57 eA-3

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#### Alert level C

PLAT029_ALERT_3_C	_diffn_measured_fraction_theta_full value Low .	0.962 Why?
PLAT068_ALERT_1_C	Reported F000 Differs from Calcd (or Missing)...	Please Check
PLAT127_ALERT_1_C	Implicit Hall Symbol Inconsistent with Explicit	-P 2ac 2n Check
PLAT213_ALERT_2_C	Atom C17 has ADP max/min Ratio .....	3.3 prolat
PLAT213_ALERT_2_C	Atom C18 has ADP max/min Ratio .....	3.2 prolat
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	18 Report
PLAT926_ALERT_1_C	Reported and Calculated R1 Differ by .....	-0.0011 Check
PLAT927_ALERT_1_C	Reported and Calculated wR2 Differ by .....	-0.0013 Check

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#### Alert level G

PLAT073_ALERT_1_G	H-atoms ref, but _hydrogen_treatment Reported as	constr Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	6.14 Why ?
PLAT128_ALERT_4_G	Alternate Setting for Input Space Group Pnam	Pnma Note
PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by ...	2 Units
PLAT300_ALERT_4_G	Atom Site Occupancy of H6A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6B Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6C Constrained at	0.5 Check
PLAT769_ALERT_4_G	CIF Embedded explicitly supplied scattering data	Please Note
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #	3 Check
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	111 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	2 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	3.0 Low
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...	4 Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	2 Info
PLAT982_ALERT_1_G	The C-f' = 0.0192 Deviates from IT-value =	0.0181 Check
PLAT982_ALERT_1_G	The Cl-f' = 0.3684 Deviates from IT-value =	0.3639 Check
PLAT982_ALERT_1_G	The F-f' = 0.0754 Deviates from IT-value =	0.0727 Check
PLAT982_ALERT_1_G	The Ir-f' = -4.3963 Deviates from IT-value =	-4.7710 Check
PLAT982_ALERT_1_G	The N-f' = 0.0326 Deviates from IT-value =	0.0311 Check
PLAT983_ALERT_1_G	The Cl-f'' = 0.6994 Deviates from IT-Value =	0.7018 Check
PLAT983_ALERT_1_G	The F-f'' = 0.0551 Deviates from IT-Value =	0.0534 Check
PLAT983_ALERT_1_G	The Ir-f'' = 6.8162 Deviates from IT-Value =	6.5667 Check

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2 **ALERT level A** = Most likely a serious problem - resolve or explain

3 **ALERT level B** = A potentially serious problem, consider carefully

8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

22 **ALERT level G** = General information/check it is not something unexpected

15 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

9 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

7 ALERT type 4 Improvement, methodology, query or suggestion

0 ALERT type 5 Informative message, check

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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.

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